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Multi-symmetric Close Packings of Equal Spheres on the Spherical Surface

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Abstract

An analysis is presented for the Tammes problem: how must n points be distributed on the surface of a sphere in order that the minimum angular distance between any two of the points be a maximum? With the analogy of the capsid structure of small 'spherical' viruses, locally extremal arrangements are constructed in tetrahedral, octahedral and icosahedral symmetry. Thirty arrangements defined by four packing sequences are investigated. By the applied construction process, novel locally extremal configurations for $n = 78$, 96, 108, 144, 150, 192, 198, 270, 360, 372, 480, 492 and improvable configurations for $n = 114$, 282 are obtained. A table is given of the investigated arrangements; most of them are putative solutions of the Tammes problem.

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Introduction

Consider the problem of the closest packing of n equal non-intersecting spheres on the spherical surface investigated by Mackay, Finney & Gotoh (1977).

This 'hard-sphere' problem, mentioned as the Fejes problem (Fejes Tóth, 1972) by Mackay, Finney & Gotoh (1977) but better known as the Tammes problem (Tammes, 1930; Fejes Tóth, 1964), has several equivalent formulations. Melnyk, Knop & Smith (1977) enumerated the different formulations of this purely geometrical problem but presented also a physical interpretation of it as an extreme case of finding equilibrium configuration where n points on the surface of a sphere repel each other according to the inverse power law. Namely, when the exponent of the power tends to infinity, the smallest distance between the points becomes dominant in the potential energy and minimizing the potential energy becomes equivalent to maximizing the smallest distance. Thus, in the limit, the problem of equilibrium configuration is equivalent to the problem of densest packing of equal spheres (or circles or spherical caps) on the sphere.

Here we will examine the Tammes problem in the form: How must n equal non-overlapping circles (spherical caps) be packed on the surface of a sphere so that the angular diameter d of the circles will be as great as possible? We chose this formulation since in this case it is easy to define the density and the graph of packing.

The density D of packing is the ratio of the total area of the surface of the spherical caps to the surface area of the sphere: $D=(n/2)[1-\cos(d/2)]$. The graph of packing is defined so that the vertices of the graph are the centres of the spherical circles and the edges of the graph are the shorter arcs of great circles joining the centres of the touching spherical circles. Thus, all the edges of the graph of a packing of equal circles are of equal length, and the length of the edges in the graph is equal to the diameter of the spherical circles.

The solution of the Tammes problem and also the extremal density of packing are known only for some values of n. For many values of n there are only estimations of the extremal density. Upper bounds can be given, for example, by Fejes Tóth's (1972) and Robinson's (1961) formulae, but lower bounds can be most appropriately given by constructions. Many construction methods have been developed for producing dense packing of equal circles on the sphere as, for example, axially symmetric packing (Goldberg, 1967), multi-branched helical packing (Székely, 1974), multi-symmetric packing (Robinson, 1969), construction of new packing by moving the graph of an existing packing (Danzer, 1963), and packing by the above-mentioned repulsion-energy minimization (Clare & Kepert, 1986).

The best packings in the literature, in general, have a moderate degree of symmetry or have no symmetry at all. This was also confirmed by a very recent paper of Clare & Kepert (1986). However, there are particular values of n ($n=4$, 6, 12, 24, 48, 120, 180) for which the proved or conjectured best packings, contrary to the general cases, have a high degree of symmetry (tetrahedral, octahedral, icosahedral). The aim of this paper is to try to extend the set of these particular cases by introducing packing sequences such that these particular packings are terms of the introduced sequences.

In this paper the multi-symmetric packing is treated in which the arrangements of the circles have rotational symmetry of the regular tetrahedron, octahedron and icosahedron. Defining an infinite family of circle packings, we shall present locally extremal arrangements for $n=78$, 96, 108, 144, 150, 192, 198, 270, 360, 372, 480, 492 and non-rigid packings for $n=114$, 282, which configurations do not seem to have been considered previously. Our investigations have been inspired by the structure of virus coats (Caspar & Klug, 1962) and Robinson's (1969) packing constructions.

Regular triangular tessellations

Consider the triangular surface lattices of 'spherical' viruses, and consider them not only on the icosahedron but also on the octahedron and tetrahedron. After Coxeter (1972), let us denote all of these regular tessellations by the symbol $\{3, q+\}_{b,c}$, where the number 3 means that the tessellation consists of equilateral triangles and the notation $q+$ refers to the fact that q or more than q (*i.e.* six) triangles meet at the vertices of the tessellation. The suffixes b, c denote the coordination numbers of triangulation.

Let us denote the number of the vertices of the tessellation $\{3, q+\}_{b,c}$ by V and the number of the vertices of the base polyhedron $\{3, q\}$ by V_r. Using the relationships of § 10.3 of Coxeter's (1969) book, we can express the number of the vertices of the tessellation (with preservation of the vertices of the base polyhedron) in the form:

$$V=T[2q/(6-q)]+2,$$

and the number of the vertices of the tessellation with removal of the vertices of the base polyhedron in the form:

$$V-V_r=(T-1)[2q/(6-q)],$$

where T is the triangulation number: $T=b^2+bc+c^2$ and $q=3, 4, 5$. These V and $V-V_r$ numbers can be considered as those values of n for which rather dense packings are expected in tetrahedral, octahedral and icosahedral rotational symmetry, but not all of them lead to a local maximum.

Robinson (1969) has constructed dense circle packings in tetrahedral, octahedral and icosahedral symmetry so that the part of the graph of the packing above a face of the polyhedron is the same in all three cases. The graphs of the circle packings obtained by him are rigid in the Danzerian sense (Danzer, 1963), which means that the edge length of the graph has a local maximum. Recently, Tarnai (1983) succeeded in applying Robinson's idea. Examining the arrangements constructed by Robinson (1969) and Tarnai (1983), one can ascertain a common property. Namely, for the tessellations $b=c+1$ or $b=c+2$ holds and the vertices of the polyhedron $\{3, q\}$ do not belong to the graph. This observation suggested that we could produce packings with the same property.

In a preliminary investigation (Tarnai, 1985) we analysed how Robinson's (1969) packings take shape when circles are packed also at the vertices of the base polyhedra $\{3, q\}$. The results obtained were not as good as the original results, but were more or less acceptable except for the arrangements in tetrahedral symmetry. So, although we did not expect very good results we decided to produce packings of this kind also.

For the calculations we have worked out a procedure which is based on the 'heating technique' (Tarnai & Gáspár, 1983) considering the graph as a spherical bar and joint structure.

Sequences of circle packings and new results

The tessellations $\{3, q+\}_{c+1,c}$ and $\{3, q+\}_{c+2,c}$ by removal and preservation of the vertices of the regular polyhedra $\{3, q\}$ define four infinite sequences of circle packings for $c = 1, 2, \ldots,$ where each term of a sequence can be defined for $q = 3, 4, 5$. In the case of preservation of the vertices of the regular polyhedra $\{3, q\}$ we only investigated the circle packings for $q = 4$ and $q = 5$. We determined the first three terms of the sequences of the circle packings, so we investigated altogether 30 arrangements.

The first sequence is defined with removal of the vertices of the base polyhedra and $b = c + 1$. So, when $c = 1$ packings for $n = 12, 24, 60$ (Robinson, 1969) are obtained; when $c = 2$ packings for $n = 36, 72, 180$ (Tarnai, 1983) are obtained; and when $c = 3$ packings for $n = 72, 144, 360$ are obtained. The subgraphs of these packings can be seen in Fig. 1 in a schematic form where (and similarly also in the forthcoming pictures) each great equilateral triangle composed of dashed lines is a face of the regular tetrahedron or octahedron or icosahedron.

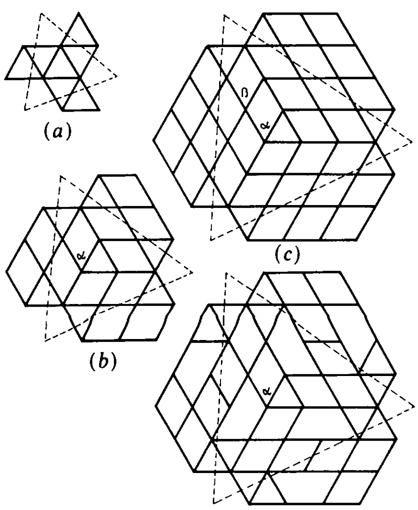

Fig. 1. Subgraph of the packing in system $\{3, q+\}_{c+1,c}$ with removal of the vertices of the base polyhedron for (a) $q = 3, 4, 5$ and $c = 1$; (b) $q = 3, 4, 5$ and $c = 2$; (c) $q = 3$ and $c = 3$; (d) $q = 4, 5$ and $c = 3$.

The second sequence is defined with removal of the vertices of the base polyhedra and $b = c + 2$. So, when $c = 1$ packings for $n = 24, 48, 120$ (Robinson, 1969) are obtained; when $c = 2$ packings for $n = 54, 108, 270$ are obtained; and when $c = 3$ packings for $n = 96, 192, 480$ are obtained. The subgraphs of these packings can be seen in Fig. 2.

The third sequence is defined with preservation of the vertices of the base polyhedra and $b = c + 1$. So, when $c = 1$ packings for $n = 30, 72$ (Tarnai, 1985) are obtained; when $c = 2$ packings for $n = 78, 192$ are obtained; and when $c = 3$ packings for $n = 150, 372$ are obtained. The subgraphs of these packings can be seen in Fig. 3.

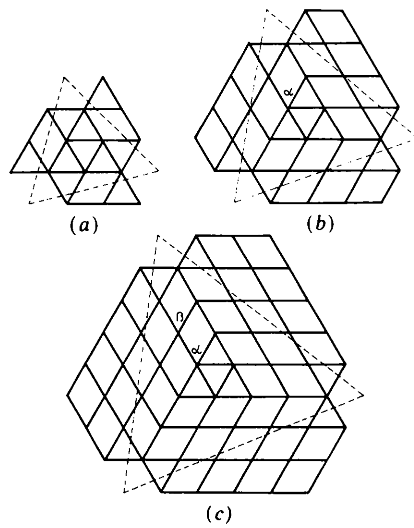

Fig. 2. Subgraph of the packing in system $\{3, q+\}_{c+2,c}$ with removal of the vertices of the base polyhedron for $q = 3, 4, 5$ and (a) $c = 1$; (b) $c = 2$; (c) $c = 3$.

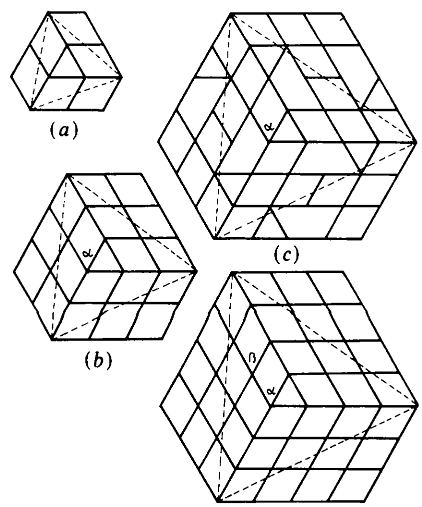

Fig. 3. Subgraph of the packing in system $\{3, q+\}_{c+1,c}$ with preservation of the vertices of the base polyhedron for (a) $q = 4, 5$ and $c = 1$; (b) $q = 4, 5$ and $c = 2$; (c) $q = 4$ and $c = 3$; (d) $q = 5$ and $c = 3$.

Table 1. *Close packings of congruent spheres on a spherical surface*

n	Tessellation	Subgraph	Diameter d (°)	Angles in the graph (°) α	β	Density D	Upper bound of maximum density	Notes
12	$\{3,3+\}_{2,1}$	Fig. 1(*a*)	63·43494			0·89609	0·89609	Robinson (1969)
24	$\{3,4+\}_{2,1}$	Fig. 1(*a*)	43·69078			0·86170	0·86170	Robinson (1969)*
30	$\{3,4+\}_{2,1}$	Fig. 3(*a*)	37·47861			0·79515	0·86304	Goldberg (1967) is better
36	$\{3,3+\}_{3,2}$	Fig. 1(*b*)	34·70342	85·22967		0·81914	0·86559	Clare & Kepert (1986) is better
48	$\{3,4+\}_{3,1}$	Fig. 2(*a*)	30·76278			0·85964	0·87105	Robinson (1969)
54	$\{3,3+\}_{4,2}$	Fig. 2(*b*)	28·27575	83·76753		0·81781	0·87349	Székely (1974)†
60	$\{3,5+\}_{2,1}$	Fig. 1(*a*)	26·82139			0·81801	0·87570	Robinson (1969)‡
72	$\{3,3+\}_{4,3}$	Fig. 1(*c*)	24·76706	93·05042	113·56839	0·83758	0·87943	$\{3,4+\}_{3,2}$, Fig. 1(*b*) is better
72	$\{3,4+\}_{3,2}$	Fig. 1(*b*)	24·85375	72·01475		0·84343	0·87943	Tarnai (1983)
72	$\{3,5+\}_{2,1}$	Fig. 3(*a*)	24·83975			0·84248	0·87943	Mackay, Finney & Gotoh (1977)§
78	$\{3,4+\}_{3,2}$	Fig. 3(*b*)	23·34706	99·41025		0·80666	0·88100	New result
96	$\{3,3+\}_{5,3}$	Fig. 2(*c*)	21·08719	92·39056	92·39056	0·81043	0·88485	New result
108	$\{3,4+\}_{4,2}$	Fig. 2(*b*)	20·20975	71·47703		0·83763	0·88686	New result
114	$\{3,4+\}_{4,2}$	Fig. 4(*b*)	18·94569	99·30375		0·77727	0·88774	The packing is not rigid
120	$\{3,5+\}_{3,1}$	Fig. 2(*a*)	19·32389			0·85109	0·88854	Robinson (1969)
132	$\{3,5+\}_{3,1}$	Fig. 4(*a*)	18·36653			0·84593	0·88997	Tarnai (1985)
144	$\{3,4+\}_{4,3}$	Fig. 1(*d*)	17·48031	76·21336		0·83609	0·89119	New result
150	$\{3,4+\}_{4,3}$	Fig. 3(*c*)	17·10933	104·58036		0·83442	0·89174	New result
180	$\{3,5+\}_{3,2}$	Fig. 1(*b*)	15·81875	64·59911		0·85617	0·89400	Tarnai (1983)
192	$\{3,4+\}_{5,3}$	Fig. 2(*c*)	15·04103	76·00683	75·86661	0·82579	0·89472	$\{3,5+\}_{3,2}$, Fig. 3(*b*) is better
192	$\{3,5+\}_{3,2}$	Fig. 3(*b*)	15·17867	75·78336		0·84095	0·89472	New result
198	$\{3,4+\}_{5,3}$	Fig. 4(*c*)	14·60186	96·76233	75·36017	0·80265	0·89506	New result
270	$\{3,5+\}_{4,2}$	Fig. 2(*b*)	12·93700	64·43083		0·85942	0·89800	New result
282	$\{3,5+\}_{4,2}$	Fig. 4(*b*)	12·44139	75·79611		0·83022	0·89835	The packing is not rigid
360	$\{3,5+\}_{4,3}$	Fig. 1(*d*)	11·20247	66·32283		0·85945	0·90010	New result
372	$\{3,5+\}_{4,3}$	Fig. 3(*d*)	10·92372	77·82400	81·65733	0·84448	0·90031	New result
480	$\{3,5+\}_{5,3}$	Fig. 2(*c*)	9·69375	66·26633	66·23108	0·85822	0·90174	New result
492	$\{3,5+\}_{5,3}$	Fig. 4(*c*)	9·46111	74·83931	66·10678	0·83799	0·90186	New result

* The packing is the same as that in $\{3,3+\}_{3,1}$, Fig. 2(*a*).
† The packing is the same as that in $\{3,4+\}_{3,1}$, Fig. 4(*a*).
‡ The packing due to Székely (1974) is better.
§ The packing in $\{3,4+\}_{3,2}$, Fig. 1(*b*), is better.

The fourth sequence is defined with preservation of the vertices of the base polyhedra and $b=c+2$. So, when $c=1$ packings for $n=54$, 132 (Tarnai, 1985) are obtained; when $c=2$ packings for $n=114$, 282 are obtained; and when $c=3$ packings for $n=198$, 492 are obtained. The subgraphs of these packings can be seen in Fig. 4.

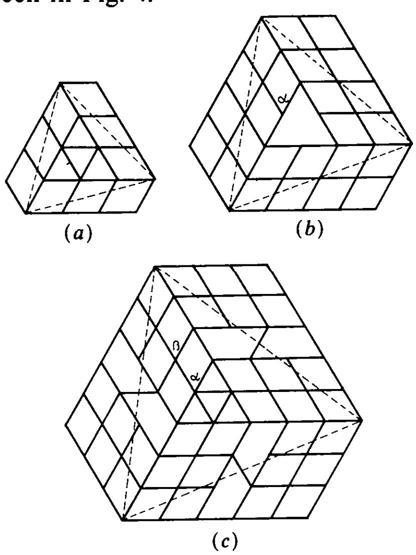

Fig. 4. Subgraph of the packing in system $\{3,q+\}_{c+2,c}$ with preservation of the vertices of the base polyhedron for $q=4$, 5 and (*a*) $c=1$; (*b*) $c=2$; (*c*) $c=3$.

The investigated packing sequences in a multi-symmetric system incorporate some known arrangements. The numerical data of these known packings and of the newly discovered packings are collected in Table 1 whose entries are arranged with increasing n. Table 1 contains the values of the density D of the actual arrangements (which are lower bounds for the extremal density) and also the upper bounds for the extremal density calculated by formula (9.5) of Robinson (1961). In order to be able to reproduce and check the results easily, in Table 1 we have given one or two angles (α, β) of the graph where the determination of these angles would be a little difficult. These angles are marked in Figs. 1 to 4. (It should be noted, however, in order that the calculation be correct, in general, a higher order of exactness is needed for the edge length d than for the angles α, β in the graph.)

Concluding remarks

It is interesting to see that 72 equal circles (spheres) can be packed on a spherical surface in arrangements different from each other in tetrahedral (Fig. 1*c*), octahedral (Fig. 1*b*) and icosahedral (Fig. 3*a*) symmetry with Danzerian rigid graphs (in each of the cases the density has a local maximum). Comparing the three cases, one can ascertain that the best result is obtained in octahedral symmetry.

Contrary to the case of $n=72$, for $n=54$ the same locally extremal packing is obtained with tetrahedral $\{3, 3+\}_{4,2}$ and octahedral $\{3, 4+\}_{3,1}$ surface lattices. It should be noted that this packing also represents a four-branched spherical helix structure (Székely, 1974; Tarnai, 1985).

The applied method did not result in Danzerian rigid packings for $n=114$ and 282. The result for $n=114$ is not of interest since the circle diameter for $n=114$ is less than the circle diameter for $n=120$. But, the arrangement of 282 circles is quite good, so it is worth improving it, by giving up the icosahedral symmetry.

Terms of the packing sequences $\{3, q+\}_{c+1,c}$, $\{3, q+\}_{c+2,c}$ defined with removal of the vertices of the base polyhedra $\{3, q\}$ present Danzerian rigid arrangements and quite large densities in all of the investigated cases. On the basis of the results obtained it is expected that Danzerian rigid packings will also be obtained in these sequences for values $c>3$.

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Theory of Electron Diffraction from Planar Ideal Crystals

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Abstract

A theory of electron diffraction from a planar ideal crystal of arbitrary thickness is presented. It is based on Schrödinger's equation. Both the relativistic corrections in energy and wavelength and the electron 'absorption' due to the presence of inelastic scattering may be incorporated as usual. This theory is constructed in an exact differential-equation approach known as rigorous coupled-wave analysis. This is an exact method of diffraction analysis that has been extensively tested for its numerical calculation scheme. The exact solution for electron wave amplitudes of all diffraction orders is formally presented in terms of a standard eigenvalue problem and explicitly expressed in matrix form. Numerical calculation can be implemented on digital computers in a straightforward manner. An approximate conservation law is given for the transmittance and reflectance, which are then the relevant dynamical quantities to be measured in a realistic time-dependent diffraction process and to be calculated in this time-independent diffraction theory for comparison. Two derivations of the well known Bragg law are sketched.

1. Introduction

In theories of electron diffraction from a planar ideal crystal, as in all wave-motion problems, the wave field is usually expanded into certain elementary waves when a differential-equation approach is adopted. The amplitudes of the elementary-wave components are to be determined, exactly or approximately, by a wave equation and boundary conditions. A particular relativistically corrected form of Schrödinger's wave equation is used when electron polarization may be ignored (Hirsch, Howie, Nicholson, Pashley & Whelan, 1977; Cowley, 1981). As for the wave expansion, there are three main types. One type is

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