An Algorithm for Generating the Sphere Coordinates in a Three-Dimensional Osculatory Packing

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Abstract. This paper develops an efficient algorithm which generates the pentaspherical coordinates of the spheres in an osculatory packing of the three-dimensional unit sphere. The algorithm has a tree-like structure and is easily modified so that, given a prescribed bound, it counts the number of spheres in the packing whose curvatures are less than this bound. The algorithm has been used to produce heuristic estimates of the exponent M of the packing, and these indicate that M is approximately 2.42.

1. **Introduction.** In a recent paper [3], we described a process for generating the pentaspherical coordinates of all the spheres in an osculatory packing of a three-dimensional unit sphere. The procedure given there is not practical because each sphere in the packing is generated infinitely often, and hence this would be a very inefficient way of actually generating the coordinates, requiring a storage of all the coordinates and a comparison of each newly generated coordinate vector with those already stored. In this paper, we present an algorithm which produces the coordinates of each sphere once and only once. Moreover, the structure of the algorithm is tree-like and hence presents no storage problems. We describe how the (theoretically infinite) algorithm can be modified to count the number of spheres in the packing of a given curvature, whose curvatures are less than a prescribed bound. The results of a computer implementation of this algorithm are given, which give heuristic estimates for the exponent M of the packing, using the technique which Melzak [5] used to estimate the two-dimensional constant S. These results indicate that $M \approx 2.42$.

2. **Preliminary Definitions and Results.** We refer the reader to [3] for a more complete explanation of the results mentioned in this section. We begin with a unit sphere (ball) U, and four open spheres $S_1, \cdots, S_4$ which are externally tangent to one another and internally tangent to U. An *osculatory packing* of U beginning with $S_1, \cdots, S_4$ is a sequence $C = \{S_n\}$ of disjoint open spheres chosen so that S_n has the largest radius of spheres contained in $U \backslash (S_1 \cup \cdots \cup S_{n-1})$, for $n = 5, 6, \cdots$. The *exponent* of the packing C is the number

$$(1) \qquad M = \sup\{t: \sum r_n^t = \infty\} = \inf\{t: \sum r_n^t < \infty\},$$

where r_n is the radius of S_n. In some cases, there is a unique such packing (up to the

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order in which spheres of equal radii are listed), and in other cases there are many such packings. Our algorithm produces a specific packing of this type, and it is known (see [3]) that M does not depend on the radii of the spheres $S_1, \cdots, S_4$. The best known estimates for M are

(2) $$2.03 < M < 2.8228 \cdots = (3 + \sqrt{7})/2.$$

See Larman [4] for the lower bound and Boyd [1] for the upper bound.

The *curvature* of a sphere is the reciprocal of its radius. We shall consider the exterior of U as a sphere X_1 with negative radius and curvature -1. We shall denote the spheres $S_1, \cdots, S_4$ alternatively by $X_2, \cdots, X_5$. Given any two spheres X and Y with radii r, s and whose centres are at distance d apart, we define the *separation* of X and Y by

(3) $$\Delta(X, Y) = (d^2 - r^2 - s^2)/2rs.$$

Then $\Delta(X, X) = -1$ and $\Delta(X, Y) = 1$, if X and Y are externally tangent. One can coordinatize any sphere Y in terms of $X_1, \cdots, X_5$ by the separation vector

(4) $$c(Y) = (\Delta(Y, X_1), \cdots, \Delta(Y, X_5))^T,$$

where the superscript T denotes transpose.

We let Δ denote the 5×5 matrix $(\Delta(X_i, X_j))$ so that $\Delta = J - 2I$, where J is the matrix all of whose entries are 1, and I is the identity matrix. We have also that

(5) $$\Delta^{-1} = 6^{-1}(J - 3I).$$

The *pentaspherical coordinate vector* of Y in terms of $X_1, \cdots, X_5$ is the vector

(6) $$a(Y) = \Delta^{-1}c(Y).$$

From $a(Y)$, one can obtain the cartesian equations of Y. Suppose X_i has centre γ_i and radius r_i, and $\xi = (\xi_1, \xi_2, \xi_3)$, and X_i has the equation $x_i(\xi) = 0$, where

(7) $$x_i(\xi) = (2r_i)^{-1}(|\xi - \gamma_i|^2 - r_i^2).$$

Then Y has the equation $y(\xi) = 0$, where

(8) $$y(\xi) = \sum \{a_i(Y)x_i(\xi): i = 1, \cdots, 5\},$$

and $y(\xi)$ has a form analogous to (7).

The curvature η of Y is determined from the curvatures $\epsilon_1, \cdots, \epsilon_5$ of $X_1, \cdots, X_5$ by

(9) $$\eta = a(Y)^T\epsilon,$$

where ϵ is the column vector $(\epsilon_1, \cdots, \epsilon_5)^T$.

The vectors $c(Y)$, $a(Y)$ and ϵ satisfy the equations

(10) $$c(Y)^T\Delta^{-1}c(Y) = -1,$$

(11) $$a(Y)^T\Delta a(Y) = -1,$$

(12) $$\epsilon^T\Delta^{-1}\epsilon = 0.$$

Equation (12) can obviously be written as

(13) $$(\epsilon_1 + \cdots + \epsilon_5)^2 = 3(\epsilon_1^2 + \cdots + \epsilon_5^2),$$

in which form it is often known as "Soddy's formula," being named after a poem by Soddy which appeared in 1936. However, the result appears in a much earlier paper (1886) by Lachlan (see [3] for precise references).

The sphere generating process described in [3] generates 5-tuples of spheres $X_1(\alpha), \cdots, X_5(\alpha)$, where α is any vector with a finite number of components, all in the set $\{1, 2, 3, 4, 5\}$. We call the set of such vectors G. By convention, G includes a single vector with no components. We let $\mathcal{G} = \{X_i(\alpha) : i = 1, \cdots, 5, \alpha \in G\}$, and $\mathcal{G}' = \mathcal{G}\backslash\{X_1\}$. Theorem 10 of [3] shows that the collection $\mathcal{G}'$ is an osculatory packing of U. For our purposes, we need only know that the pentaspherical coordinates of the spheres $X_1(\alpha), \cdots, X_5(\alpha)$ are given by the five columns of a matrix $A(\alpha)$ whose calculation we will now describe. Let e_i $(i = 1, \cdots, 5)$ be the column vector with all components zero except for a 1 in the ith position, and let e be a vector with all components 1. Let $A_i, i = 1, \cdots, 5$, be the following matrices:

$$A_1 = (e_2, e_3, e_4, e_5, e - 2e_1),$$

$$A_2 = (e_1, e_3, e_4, e_5, e - 2e_2),$$

(14) $$A_3 = (e_1, e_2, e_4, e_5, e - 2e_3),$$

$$A_4 = (e_1, e_2, e_3, e_5, e - 2e_4),$$

$$A_5 = (e_1, e_2, e_3, e_4, e - 2e_5).$$

If $\alpha = (i_1, \cdots, i_m) \in G$, then

(15) $$A(\alpha) = A_{i_1} \cdots A_{i_m}.$$

Note that the entries of the A_i and hence $A(\alpha)$ are integers. The columns of $A(\alpha)$, by Lemma 2 of [3], are the pentaspherical coordinates of $X_1(\alpha), \cdots, X_5(\alpha)$.

In order to generate $\mathcal{G}$ as efficiently as possible, we wish to produce an algorithm which will generate each $X \in \mathcal{G}$ once and only once. Observing the formation of the matrices A_i, we see that if $(\alpha, i) = (i_1, \cdots, i_m, i)$, then the sets $(X_1(\alpha), \cdots, X_5(\alpha))$ and $(X_1(\alpha, i), \cdots, X_5(\alpha, i))$ have four spheres in common, and $X_5(\alpha, i)$ is a "new" sphere. Thus, apart from the initial spheres $X_2, \cdots, X_5$, we need only generate the spheres $X_5(\alpha)$ for each $\alpha \in G$. It can be shown, with some effort, that the spheres $X_5(\alpha)$, with α having components only in the set $\{1, 2, 3\}$, are all distinct. However, $A_4^6 = I$ and $A_5^2 = I$; so there are many relations, in general, of the form $X_5(\alpha) = X_5(\beta)$, with $\alpha \neq \beta$, $\alpha, \beta \in G$. Hence, the "natural" algorithm which would produce all $X_5(\alpha)$ with $\alpha \in G_m$, successively, for $m = 1, 2, \cdots$, would be extremely inefficient. Furthermore, in practice, one wants an algorithm which produces all $X_5(\alpha)$ whose curvatures lie below some prescribed bound, and the wide variation in curvatures among the $X_5(\alpha)$ with $\alpha \in G_m$, for some particular m, would make this naive method even more unsuitable.

3. An Efficient Algorithm. In this section, we describe an algorithm which produces all the desired coordinates once and only once. We begin with a preliminary version (Lemma 1) which is not quite as efficient as the final version described in Theorem 2, since it produces some coordinates twice. However, with the preliminary algorithm, it is quite easy to see that *all* coordinates are produced, while this would not be as obvious for the improved algorithm.

Let $\mathcal{K}$ denote the set of coordinate vectors $a(X)$ for $X \in \mathcal{G} = \{X_i(\alpha) : i = 1, \cdots, 5, \alpha \in G\}$. It is easily seen that if a is in $\mathcal{K}$, then any vector a', whose components are permutations of the components of a, is also in $\mathcal{K}$. In particular, if a^* is the rearrangement of a into decreasing order, then a^* is in $\mathcal{K}$. Hence, it suffices to generate only those vectors whose components are in decreasing order, and we denote this set of vectors by $\mathcal{K}^*$. If $w \in \mathcal{K}^*$, we shall write

$$(16) \qquad\qquad U_i w = (A_i w)^*,$$

so that $U_i w$ has components $w_j + w_i$ $(j \neq i)$ and $-w_i$, arranged in decreasing order.

It is clear that each $w \in \mathcal{K}^*$ is of the form $w = U_{i_1} \cdots U_{i_m} e_1$, where $i_1, \cdots, i_m$ are suitable integers in $\{1, \cdots, 5\}$. We may now think of generating $\mathcal{K}^*$ as a list, in the following way: We begin with e_1, then add to our list $U_5 e_1, \cdots, U_1 e_1$, then repeat with each of the new vectors in our list, and so on. However, if w is in the list and $w_i = 0$, it is clear that $U_i w = w$, so we need not apply U_i. Also if $w_i = w_{i+1}$, we need not apply U_i. Finally, if $x = U_j w$ has just been obtained, and $x_i = -w_j$, then $U_i x = w$, so we need not apply U_i to x. We shall see in Lemma 1 that we need never apply U_i to w if $w_i < 0$. This will mean U_5 is never used.

The reader may verify that the following is the beginning of the list which we obtain (writing the coordinate vectors now as row vectors):

1	0	0	0	0	(0)
1	1	1	1	−1	(1)
2	2	2	0	−1	(2)
4	4	2	1	−2	(3)
5	5	3	−1	−1	(4)
6	6	3	0	−2	(4)
8	6	5	2	−4	(4)

The number in parenthesis indicates the number of operations U_i required to obtain the given vector.

LEMMA 1. *Let $U_1, \cdots, U_5$ be the operations described in the above paragraphs. Given any vector $w = (w_1, \cdots, w_5)$, with $w_1 \geqq \cdots \geqq w_5$, we say that U_i is admissible for w, if $w_i > 0$ and $w_i > w_{i+1}$. Let $U(w)$ be the set of (at most five) vectors $U_i w$ such that U_i is admissible for w. Let $P_0 = \{(1, 0, 0, 0, 0)\}$, and $P_n = U(P_{n-1})$ for $n = 1, 2, \cdots$. Then, for $n \geqq 1$,*

   (a) *if $w \in P_n$, then $w_1 \geqq w_2 \geqq w_3 > 0 > w_5$;*

   (b) *for each $w \in P_n$, if $w_4 \geqq 0$ or if $0 > w_4 = w_5$, then there is a unique $u \in P_{n-1}$ and a unique i so that U_i is admissible for u and $U_i u = w$;*

   (c) *if $w \in P_n$ and $0 > w_4 > w_5$, then there are exactly two vectors $u, v \in P_{n-1}$, and corresponding i, j so that $w = U_i u$ and $w = U_j v$;*

   (d) *if $m, n \geqq 0$, and $m \neq n$, then P_m and P_n are disjoint.*

   Proof. We shall give the proofs by induction, proving (d) in the form that $P_m \cap P_n = \varnothing$ if $m < n$. The results are true, by inspection, if $n = 1$. To prove (a) for P_n, let $w \in P_n$, and $w = U_i u$ with $u \in P_{n-1}$ and U_i admissible for u. Then $u_i > 0$, and the components of w are $u_j + u_i$ $(j \neq i)$ and $-u_i$ in decreasing order. Since

(a) holds for u (by induction), we at least have $w_1 \geqq w_2 > 0$, so $-u_i$ is one of w_3, w_4 or w_5. Now, by checking all possibilities for i, we can see that

$$(17) \qquad w_3 + w_4 + w_5 \geqq u_3 + u_4 + u_5.$$

Then it follows by induction that $w_3 + w_4 + w_5 \geqq 1$, and hence certainly $w_3 > 0$. Since at least one component of w (namely $-u_i$) is negative, certainly $w_5 < 0$.

To prove (b), let w, u, i be as above. By assumption, w has but one distinct negative component, so it must be $-u_i$. That is, $w_5 = -u_i$ and the other components of u must be $w_1 + w_5$, $\cdots$, $w_4 + w_5$. Since u is in decreasing order, u is determined uniquely. The number i is also unique since $U_j u = U_i u$ for $j < i$ would contradict the admissibility of U_i for u.

To prove (c), suppose $w = (a, b, c, -d, -e)$, where $0 < d < e$. We find, by extending the list preceding this lemma that n must be $\geqq 6$. There are two possibilities (and we show both hold).

   (i) $d = u_i$ for some $u \in P_{n-1}$,
   (ii) $e = v_j$ for some $v \in P_{n-1}$.
If (i) holds, then

$$u = (a - d, b - d, c - d, d, -d - e)^* \in P_{n-1}.$$

By (b) or (c) for u, u has a predecessor in P_{n-2} which we may take to be

$$u' = (a - 2d - e, b - 2d - e, c - 2d - e, d + e, -e)^* \in P_{n-2},$$

and, by the same argument, $u' \in U(u'')$, where

$$u'' = (a - 2d - 2e, b - 2d - 2e, c - 2d - 2e, d, e)^* \in P_{n-3}.$$

The vector u'' is symmetric in d and e; however, we can obtain successively

$$v' = (a - d - 2e, b - d - 2e, c - d - 2e, d + e, -d)^* \in U(u'') \subset P_{n-2}$$

and

$$v = (a - e, b - e, c - e, e, -e - d)^* \in U(v') \subset P_{n-1}.$$

Finally, we see that $w \in U(v)$. Note that $u \neq v$, for if $u = v$, then since $d \neq e$, we must have d equal to one of $a - e$, $b - e$ or $c - e$. If, say, $d = a - e$, then $b - e = c - d$ and $c - e = b - d$ are the only possibilities and together these imply $d = e$, a contradiction. Since w has clearly *at most* two predecessors in P_{n-1}, we have proved (c).

Finally, to prove (d), we observe that if $w \in P_n$, $n \geqq 1$, then $w_5 < 0$, so $P_n \cap P_0 = \varnothing$. Now, we use induction on m to show $P_m \cap P_n = \varnothing$ if $m < n$. For, if $w \in P_n \cap P_m$, then, by (b) or (c), $w \in U(u)$, where $u \in P_{n-1}$ and also $u \in P_{m-1}$. Thus $P_{n-1} \cap P_{m-1} \neq \varnothing$, a contradiction of the induction assumption.

THEOREM 2. *For any vector* $w = (w_1, \cdots, w_5)$, *let* T_i $(i = 1, \cdots, 4)$ *be the* (linear) *mapping which maps* w *into the vector* w', *where*

$$
\begin{aligned}
w'_j &= w_j + w_i \qquad &&\text{if } j < i, \\
&= w_{i+1} + w_i \qquad &&\text{if } i \leqq j < 5, \\
&= -w_i \qquad &&\text{if } j = 5.
\end{aligned}
$$

We say that T_i is admissible for w under the following circumstances:
    (i) *if $i = 1, 2, 3$, we require $w_i > w_{i+1}$,*
    (ii) *if $i = 4$, we require $2w_4 + w_5 \geqq 0$ and $w_4 > 0$.*
Let $T(w)$ be the set of (at most four) vectors $T_i w$ such that T_i is admissible for w. Let $Q_0 = \{(1, 0, 0, 0, 0)\}$ and $Q_n = T(Q_{n-1})$ for $n = 1, 2, \cdots$. Then $Q_n = P_n$ ($n = 0, 1, \cdots$), where P_n is as in Lemma 1. Also, for each $w \in Q_n$, there is a unique $u \in Q_{n-1}$ and a unique i for which T_i is admissible for u and $w = T_i u$.

    Suppose that $X \in \mathcal{G}$ and has the coordinate vector $a = a(X)$. Then, there is a unique n and $w \in Q_n$ such that $a^* = w$. Furthermore, for any n, if $w \in Q_n$, then all distinct permutations of w are coordinate vectors of spheres in $\mathcal{G}$.

    Proof. We shall show that $Q_n = P_n$ of Lemma 1. This is clearly true for $n = 0$ and we proceed by induction. Suppose $w \in Q_n$ and $w = T_i u$, with $u \in Q_{n-1} = P_{n-1}$, and T_i is admissible. Then we claim $T_i u = (T_i u)^* = U_i u$. We need only show that $w_5 \leqq w_4$. This holds if and only if $2u_i + u_5 \geqq 0$. For $i = 4$, this is part of requirement (ii) and for $i = 1, 2, 3$ it follows from $u_3 + u_4 + u_5 \geqq 1$ proved in Lemma 1, since

$$2u_i + u_5 \geqq u_i + u_4 + u_5 \geqq u_3 + u_4 + u_5$$

for $i = 1, 2$ or 3.

    Hence, we have $Q_n \subset P_n$. To show equality, suppose $w \in P_n$. Then by Lemma 1 (b), (c), W has one or two predecessors in $P_{n-1} = Q_{n-1}$. In either case, one of the predecessors is

$$u = (w_1 + w_5, \cdots, w_4 + w_5, -w_5)^*,$$

and, if $u_i = -w_5$, then $2u_i + w_5 = w_4 - w_5 \geqq 0$, and $u_i > 0$, so that if i is chosen maximally, T_i is admissible for u, and so $w = T_i u \in Q_n$. It is easy to see that (ii) rules out the other possible predecessor for w, so w has a unique predecessor in Q_{n-1}.

    Finally, our remarks at the beginning of this section prove the final statement of the theorem.

    Remarks. 1. We shall call the set of spheres whose coordinates are rearrangements of a vector in $P_n = Q_n$ the nth generation of spheres. It is clear that n is the minimal integer for which $X \in \mathcal{G}$ has a representation as $X_i(\alpha)$ where α has n components.

    2. There are certain aspects of the algorithm described in Theorem 2 which are of importance in practice. We may assume that the curvatures $\epsilon_1, \cdots, \epsilon_5$ of $X_1, \cdots, X_5$ satisfy $-1 = \epsilon_1 < \epsilon_2 \leqq \cdots \leqq \epsilon_5$. In addition to the vector ϵ, we use the vector $\kappa = \Delta^{-1}\epsilon$ which has components

(18) $$\kappa_i = (\epsilon_1 + \cdots + \epsilon_5 - 3\epsilon_i)/6.$$

According to (9) and (6), the curvature $\epsilon(X)$ of a sphere X is given by

(19) $$\epsilon(X) = a(X)^T \epsilon = c(X)^T \kappa.$$

We shall assume always that $\kappa_j \geqq 0$ for all j. The geometrical meaning of this is that the centre of U lies in the convex hull of the centres of $X_2, \cdots, X_5$. We claim that this condition implies that if $u \in P_n$ ($n \geqq 1$) is the coordinate vector of a sphere X, and $w = T_i u$ (with T_i admissible) corresponds to a sphere Y, then the curvatures of Y and X satisfy

(20) $$\epsilon(Y) \geqq \epsilon(X).$$

To see this, one notes that $c(X)$ and $c(Y)$ are vectors with components which are integers ≥ 1 (since $X \in \mathcal{G}$ is not one of $X_1, \cdots, X_5$ so $\Delta(X, X_i) \geq 1$). By direct computation,

$$
\begin{aligned}
(21) \qquad c_j(Y) &= c_j(X), & 1 \leq j < i, \\
&= c_{j+1}(X), & i \leq j < 5, \\
&= c_i(X) + 6u_i, & j = 5,
\end{aligned}
$$

so that $c_j(Y) \geq c_j(X)$ for all j, from which (20) follows.

Also, note that if $u \in P_n$, then the set $T(u)$ represents the coordinates of up to $480 = 4 \times 5!$ spheres of $\mathcal{G}$, corresponding to the admissible $T_1, \cdots, T_4$ and the distinct permutations of each T_iw. We claim that, of these spheres, the one with least curvature is that with components T_iu, where i is the largest value for which T_i is admissible. To see this, note that $w = T_iu$ is in decreasing order, so if σ is any permutation of $\{1, \cdots, 5\}$, then $\epsilon_1 \leq \cdots \leq \epsilon_5$ implies

$$
(22) \qquad \epsilon_1 w_1 + \cdots + \epsilon_5 w_5 \leq \epsilon_1 w_{\sigma(1)} + \cdots + \epsilon_5 w_{\sigma(5)}.
$$

Also, if $j < i$, and T_j is admissible, and if Y and Z are the spheres corresponding to T_iu and T_ju, respectively, then (21) shows that

$$
(23) \qquad \epsilon(Y) \leq \epsilon(Z).
$$

In practice, one does not permute the vector w, but rather, permutes the curvatures ϵ_i since this need be done only once. The various vectors w are weighted as appropriate for the number of distinct permutations. For $n \geq 3$, if $w \in P_n$, it can be shown that there are only three possibilities; either $w_1, \cdots, w_5$ are distinct or else there is one equal pair of w_i or else two such pairs.

3. We mentioned earlier that the algorithm has a tree-like structure. In other words, each w in $\bigcup P_n$ has a *unique* representation in the form

$$
w = T_{i(n)} \cdots T_{i(1)}e_1,
$$

where $T_{i(k)}$ is admissible for $T_{i(k-1)} \cdots T_{i(1)}e_1$ for each $k = 1, \cdots, n$. Thus, one can imagine an infinite tree: The nodes at height n correspond to the vectors w in P_n; edges lead from a w in P_n to the vectors in $T(w)$ in P_{n+1}. Assigned to each node w in the tree is the number $w^T\epsilon = \epsilon_1 w_1 + \cdots + \epsilon_5 w_5$ corresponding to the least curvature of the spheres corresponding to that node (by (22)). We set an index $f(n)$ for each level initially at 4 for all n, and generate successively $w_0 = e_1, T_{i(0)}w_0 = w_1, T_{i(1)}w_1 = w_2, \cdots$ where $i(n)$ is the largest $i \leq f(n)$ for which T_i is admissible for w_i. Once $T_{i(n)}$ has been used, we set $f(n) = i(n) - 1$. To determine the number of spheres $W(m)$ for which $m \leq w^T\epsilon < m + 1$ for all integers $m \leq B$, say, we proceed upward until $w_n^T\epsilon > B$. With each new node generated, we increase $W(m)$ by 1 for each sphere corresponding to this node which has curvature η, with $[\eta] = m$. Once $w_n^T\epsilon > B$, we reduce n and proceed upward along a new branch corresponding to $f(n)$. If $f(n) = 0$, we reduce n further. Eventually, this will generate all spheres. Notice that we need provide storage only for N coordinate vectors, where N is such that for $n \geq N$, $w^T\epsilon > B$ for all $w \in P_n$. The value of N is quite small, of the order of magnitude of $\sqrt{B}$.

4. Results of a Computer Study. Using Theorem 2 and the succeeding remarks, we wrote a computer programme in FORTRAN which counts the number $W(C)$ of spheres in the packing $\mathcal{G}'$ which have the integer part of their curvature equal to C for all $C \leqq \text{CMAX}$, where CMAX is prescribed, as are $\epsilon_1 = -1$, $\epsilon_2, \cdots, \epsilon_5$ satisfying (13), and with $\kappa_j \geqq 0$, where κ_j is given by (17). Using the values of $W(C)$ so obtained, a linear law in $\log C$ is fitted to the cumulative sum $\log (\sum W(i) : i \leqq C)$ by using least squares. In this way, one obtains an approximate relation

$$(24) \qquad |\{ X \in \mathcal{G}' : \epsilon(X) \leqq C \}| \approx AC^{-M'},$$

where M' should be an approximation to M. In [5], Melzak used a similar method to estimate the two-dimensional packing constant S and obtained the heuristic result

$$(25) \qquad S \approx 1.306951.$$

Since this author has recently [2] shown rigorously that

$$(26) \qquad 1.300197 < S < 1.314534,$$

the method would seem quite reliable.

For the initial choice of curvatures $(-1, 2, 2, 3, 3)$, suggested by Soddy's "bowl of integers" [6], the curvatures of all spheres are clearly integers. In this packing, the two spheres of curvature 2 are tangent along a diameter of U and six spheres of curvature 3 touching U and the two spheres of curvature 2 can be arranged in a ring around the central spheres. (This corresponds to the matrix relation $A_4^6 = I$.) Thus, the packing $\mathcal{G}'$ is unchanged by a rotation through $\pi/3$ about the diameter common to X_1, X_2 and X_3. This means that $W(C)$ is divisible by 6 for all $C > 2$, which is a good check on the computations. For CMAX = 300, the running time on the IBM 360/65 at the University of British Columbia was 135 seconds. The total number of spheres, with curvature C at most 300, is 305,594 and these occupy .94727 of the volume of U. The values of A and M' of (24) are $A_1 = .2988455$ and

$$(27) \qquad M_1 = 2.42009.$$

An interesting point is that in this packing the curvature of each sphere satisfies $C \equiv 0, 2 \pmod 3$. This is easily proved once it is noted (by induction) that all coordinate vectors in $\bigcup P_n$, modulo 3, are rearrangements of one of the three types $(1, 1, 1, 1, 2)$, $(0, 2, 2, 2, 2)$ or $(0, 0, 0, 0, 1)$. The number N mentioned in Remark 3 of the previous section (the "height of the tree") was 38. Much information was printed out which is not reproduced here. In particular, the 300 values $W(C)$ were printed, and the numbers of spheres of curvature at most 300 in each generation P_n, $n = 1, \cdots, 38$, were printed.

In another run with initial curvatures $(-1, 2, 2, 3, 3)$ and CMAX = 100, we produced a list in lexicographic order of the coordinate vectors w, and the corresponding separation vectors.

Another interesting set of initial curvatures is $(-1, a, a, a, a)$ where $a = 1 + \sqrt{6}/2$. This corresponds to a configuration in which $X_2, \cdots, X_5$ have their centres at the vertices of a regular tetrahedron. With CMAX = 600, running time was 94 seconds. There were 1,693,595 spheres counted, distributed into 49 generations. The values of A and M' were $A = .3149755$ and

(28) $M_2 = 2.41748$.

From (27) and (28), it seems reasonable to expect that $M \approx 2.42$. A rigorous justification of this would be of considerable interest. Even more interesting would be a rigorous justification of the method itself, but this would seem to present considerable difficulties.

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