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On the Sphere Packing Problem

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Introduction. In discrete geometry and in solid state mathmatical physics we often consider problems with the symmetry of a Lie group G of invariance transformations, but admitting only discrete solutions.

It is a heuristic principle to guide our search for optimal distributions (in some well defined sense) that among them there will be some that participate in the symmetry of the problem by means of a 'large' discrete symmetry group of the distribution contained in G.

Here 'large' can mean: 'a discrete group of G with compact left coset space' or a discrete group H of G with positive, but finite Haar measure of a suitable left representative set of G modulo H.

For example for the sphere packing problem in the euclidean 3-dimensional space E_3 G is the Galilei transformation group $\mathcal{E}_3$ of 6 parameters.

A candidate for an optimal density arrangement of solid unit spheres in the E_3 without overlapping is any hexagonal 3-lattice with minimal distance 1 between distinct lattice points. Its symmetry group is a space group with the lattice translations as translation subgroup and a point group of order 24 being the direct product of the tetrahedral rotation group with the central inversion group of order 2 in any lattice point.

Its left coset factor space in $\mathcal{E}_3$ is compact.

The Problem. Ask almost anybody but a mathematician how he would pack as many oranges as possible in a crate; he will answer you about as follows: place an hexagonal layer as in Fig. 1

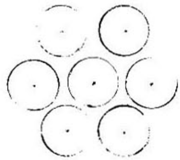

Figure 1

on the bottom, place on top of it another hexagonal layer by making use of the groves formed by the first layer and continue until the crate is filled.

For the mathematical treatment of the packing problem we idealize the shape of an orange as a solid sphere of fixed positive radius r in the euclidean space E_3 of dimension 3.

Any pointset S of the E_3 satisfying the admissibility condition

$$(1) \qquad \forall(p,q)(p \in S \ \& \ q \in S \ \& \ p \neq q \Rightarrow \overline{pq} \geq 2r)$$

is said to define an r-sphere packing consisting of the solid spheres

$$(2) \qquad \sigma_r(p) = \{q \mid q \in E_3 \ \& \ \overline{pq} \leq r\}$$

of radius r centered at the points r of S.

We observe that (1) is the necessary and sufficient condition that any two solid spheres (2) centered at points of S have no inner point in common; they do not overlap.

If the point set S is bounded then it is finite.

For any bounded subset B of the E_3 the maximum cardinality of a pointset S satisfying the admissibility condition (1) as well as the containment condition

(3) $\sigma_r(p) \subseteq B \quad (p \in S)$

is a non-negative rational integer $P(B,r)$, the <u>sphere packing number</u> of B .

It remains unchanged upon application of any rigid motion to B . This is because the application of an isometry

(4)
$$\begin{aligned} &(A,t) : E_3 \to E_3 \\ &\overrightarrow{O((A,t)(p))} = A(\overrightarrow{Op}) + t \\ &(O = (0,0,0),\ A \in \mathbb{R}^{3x3} \quad \& \quad AA^T = I_3\ ,\ t \in \mathbb{R}^{1x3}) \end{aligned}$$

of the E_3 carries a solid sphere of radius r into another solid sphere of E_3 . Note that any isometry of E_3 is of the form (4) and that the isometries of E_3 form a six parametric Lie group $\mathbb{E}_3$, the symmetry group of the sphere packing problems.

The Frobenius symbol (A,T) denoting an isometry of the E_3 consists of two parts, the <u>homogenous</u> part A and the <u>translative</u> part t . The mapping

$$\begin{aligned} &H : \mathbb{E}_3 \to O(3) \\ &H((A,t)) = A \end{aligned}$$

provides an epimorphism of $\mathbb{E}_3$ on the full orthogonal group of degree 3 the kernel of which is the abelian <u>translation group</u> Π_3 formed by the translations (E,t) by the 3-vectors t . The mapping

$$(E,t) \mapsto t \qquad (t \in \mathbb{R}^{1\times 3})$$

provides an isomorphism of the 3-translation group $\mathbb{T}_3$ and the 3-vector space $\mathbb{R}^{1\times 3}$.

We denote the group of the isometries of a metric space S by IS(S), e.g.

$$(5) \qquad IS(E_3) = \mathbb{E}_3 \quad .$$

Any non-empty subset S of E_3 is a metric space. The isometries of E_3 carrying S on S form a subgroup $IS(E_3,S)$ of $\mathbb{E}_3$ said to be the <u>symmetry group</u> of S . The restriction mapping

$$(6) \qquad \begin{aligned} &res_S : IS(E_3,S) \to IS(S) \\ &res_S(\alpha)(p) = \alpha(p) \qquad (p \in S) \end{aligned}$$

provides an epimorphism of $IS(E_3,S)$ on $IS(S)$ the kernel of which is formed by the isometries of E_3 that leave the linear manifold generated by S pointwise fixed.

Denoting by $\rho = \dim S$ the $\mathbb{R}$-linear dimension of that linear manifold it follows that $\ker res_S$ is isomorphic to the full orthogonal group of degree $3 - \rho$:

$$(7) \qquad \ker res_S \simeq O(3 - \dim S)$$

The non-degenerate <u>similarity mappings</u> of the E_3 form an overgroup IT_3 of $\mathbb{E}_3$. It is a 7-parametric Lie group generated by $\mathbb{E}_3$ and by the <u>central dilatations</u>

(8a) $$\bar{\lambda} : E_3 \to E_3$$
$$\bar{\lambda}((\xi_1,\xi_2,\xi_3)) = (\lambda\xi_1,\lambda\xi_2,\lambda\xi_3) \qquad ((\xi_1,\xi_2,\xi_3) \in E_3 \; ; \; \lambda \in R) \; .$$

Any bounded point set B is carried into the bounded pointset

(8b) $$\bar{\lambda}B = \{\bar{\lambda}(p) \mid p \in B\} \quad .$$

Since the packing number $P(B,r)$ is a rational integer, in general the function $P(\bar{\lambda}(B),r)$ will be not continuous. We remedy this situation as follows. For any pointset S satisfying the admissibility condition (1) form the pointset $A(S,B,r)$ obtained as the union of the intersection of the solid sphere $\sigma(p,r)$ $(p \in S)$ centered at the points of S with the closure $\bar{B}$ of B.

The Lebesgue measure $\mu A(S,B,r)$ of the bounded closed pointset $A(S,B,r)$ is bounded. Form the least upper bound $A(B,r)$ of the numbers

(9) $$\mu A(S,B,r) \cdot 3/4\Pi r^3$$

for all sphere packing pointsets S satisfying (1).

The number $A(B,r) = A(\bar{B},r)$ is now a non-negative number depending on B and r which is invariant under the isometries of E_3.

Note that the numerical factor $3/4\Pi r^3$ is the inverse of the volume of a solid sphere of radius r. A <u>best sphere packing</u> of B is any sphere packing for which $\mu A(S,B,r) \cdot 3/4\Pi r^3 = A(B,r)$. Two sphere packings S, S' of B are said to be equivalent if they determine the same subset of $\bar{B}$ as union of the intersection of the solid spheres $\sigma(p,r)$ centered at the points of S, S' respectively. This equivalence has of course the 3 properties of an equivalence relation.

If the pointset B is convex then $A(B,r)$ and $P(B,r)$ differ from each other only by an amount in the order of magnitude of the surface of B.

In other words, for the treatment of the packing problem we will allow even to pack <u>sections</u> of whole oranges as long as there is no overlapping of any two oranges.

Let us now briefly summarize the properties of <u>lattices</u>.

A (geometric) <u>lattice</u> of the E_3 is defined as a non-empty discrete subset of the E_3 satisfying the <u>parallelogram condition</u> (see Fig. 2)

(10) $$\forall(p,q,r,s)(p \in L \,\&\, q \in L \,\&\, r \in L \,\&\, s \in E_3 \,\&\, \overrightarrow{rs} = \overrightarrow{pq} \Rightarrow s \in L)$$

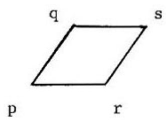

Fig. 2

For any lattice L of the E_3 the vectors $\overrightarrow{pq}$ from a fixed point p of $\vec{L}$ to an arbitrary point q of L form a module $\vec{L}$ under vector addition. The module $\vec{L}$ is an additive free abelian group of rank $\rho \leq 3$ independent of the choice of p. Thus there is a generator set $b_1,\ldots,b_\rho$ of L. Any such set is said to be a <u>basis</u> of $\vec{L}$. It is linearly independent over the real number field $\mathbb{R}$ and it spans $\vec{L}$ over the rational integer ring $\mathbb{Z}$.

Conversely, for any point p of the E_3 and for any set of linearly independent elements $b_1,b_2,\ldots,b_\rho$ of the 3-vector space $\mathbb{R}^{1\times 3}$ the pointset

(11) $$L = L(p;b_1,b_2,\ldots,b_\rho) = \{q \mid \vec{pq} \in \sum_{i=1}^{\rho} \mathbb{Z}\, b_i\}$$

forms a ρ-lattice emanating from p . The rank $\rho = \dim(L)$ of $\vec{L}$ depends on L only and is said to be the dimension of L .

If the demension ρ is positive then the transition from one basis $b_1,b_2,\ldots,b_\rho$ to another one, say $b_1',b_2',\ldots,b_\rho'$ is defined by means of a unimodular matrix

(12a) $$U \in GL(\rho,\mathbb{Z})$$

such that

(12b) $$B' = UB$$

where B is the ρx3-matrix with row vectors $b_1,\ldots,b_\rho$ and B' is the ρx3-matrix with row vectors $b_1',\ldots,b_\rho'$. The real number

(13) $$\|L\| = \|\vec{L}\| = |(\det BB^T)^{1/2}|$$

is a positive number depending only on L called the mesh of L .

Among the symmetries of a point lattice L there are the lattice translations (E,x) with x in $\vec{L}$. They are the only translations belonging to the symmetry group of L . All isometries of a lattice form a symmorphic space group. Its point group consists of all isometries of L fixing one of the points of L . Among them there is always the inversion at that point. A lattice L is said to be hexagonal if it is of positive dimensions, and if it has a basis $b_1,b_2,\ldots,b_\rho$ with the property that all basis vectors have the same length λ and that any two of them include the angle of 60^o between them

(14) $\quad b_i b_i^T = \lambda^2 \quad (1 \leq i \leq \rho)$

$$b_i b_k^T = \lambda^2/2 \quad (1 \leq i < k \leq \rho)$$

(s. Fig. 3 showing a plane hexagonal lattice)

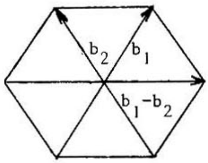

Fig. 3

There are precisely $\rho \cdot (\rho + 1)$ lattice vectors of length λ viz.

(15) $\quad \pm b_i, \pm(b_j - b_k) \quad (1 \leq i \leq \rho,\ 1 \leq j < k \leq \rho)$

all other non-zero lattice vectors are of length $>\lambda$. Any hexagonal lattice of shortest length λ is admissible with respect to sphere packing of radius $r \leq \lambda/2$.

The mesh of a ρ-dimensional hexagonal lattice of shortest length λ equals $\sqrt{\rho + 1}(\lambda^2/2)^{\rho/2}$.

The point symmetry group of the hexagonal ρ-lattice is the direct product of the inversion group and the group generated by the ρ reflections in $b_1, b_j - b_{j-1} \quad (1 < j \leq \rho)$. The latter group ist the Coxeter group with the symbol

o---o---o ... o---o

of ρ vertices isomorphic to the symmetric permutation group of $\rho + 1$ letters.

It is claimed that for regular tetrahedral crates of side length $\kappa > 0$

$$(16a) \qquad T(\kappa) = \{ \sum_{i=1}^{4} \xi_i a_i \mid \xi_i \in R$$

$$\& \ 0 \leq \xi_i \qquad (1 \leq i \leq 4)$$

$$\& \ \sum_{i=1}^{4} \xi_i = \frac{\sqrt{6}\,\kappa}{4} \}$$

with

$$(16b) \qquad \begin{aligned} a_1 &= (1,1,1) \\ a_2 &= (1,-1,-1) \\ a_3 &= (-1,1,-1) \\ a_4 &= (-1,-1,1) \end{aligned}$$

there is precisely one best sphere packing up to equivalence viz. the one provided by the hexagonal lattice

$$L(r) = L(0; \sum_{i=1}^{4} \frac{2r}{\sqrt{3}} \mathbf{Z}\, a_i) \quad .$$

In other words

$$(17) \qquad A(T(\kappa),r) = \mu A(L(r),T(\kappa),r) \cdot 3/4\Pi r^3$$

The solution: For this purpose one develops an infinitesimal calculus following Study's ideas. The symmetry group of the regular tetrahedron is used in a decisive manner. The result (17) implies the validity of the statement made in the beginning.