Close lattice packings

Problem statement

Find out how "densely" a large number of objects can be packed together.

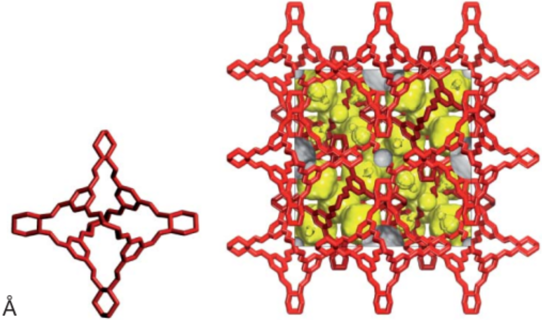
Alternatively, what is the greatest number of objects that can be packed in a predefined region.

Motivation

Crystal structure prediction

Packings of molecules in crystals

CC3



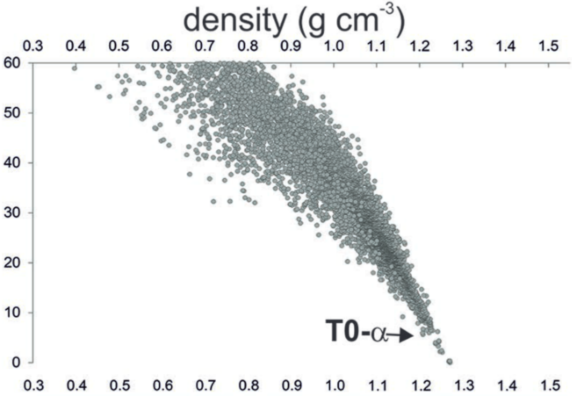
J. T. A. Jones et al., Modular and predictable assembly of porous organic molecular crystals, Nature vol. 474, p. 367–371, 2011.

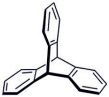
Crystal structure prediction

Observation

Crystals with lowest energy seem to form close packings.

T0

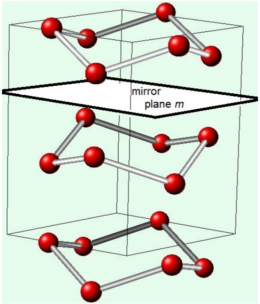




T0

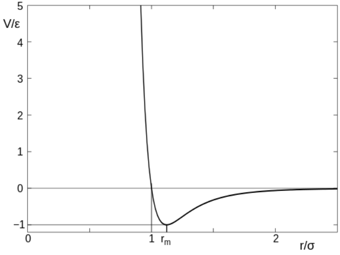
G. M. Day, A. I. Cooper, Energy-Structure-Function Maps: Cartography for Materials Discovery, Adv. Mater.,vol. 30, p. 1704944, 2018.

- optimisation of lattice energy based on space group symmetries
- energy calculations based only on intermolecular interactions
- DFT is used for more precise energy calculations



$$V_{\text{LJ}}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- ϵ - Lennard-Jones potential well depth
- σ - the finite distance at which the inter-particle potential is zero
- r - the distance between the particles



Crystal structure prediction

Lennard-Jones potential stationary points

$$V_{\mathrm{LJ}} = 4\epsilon \sum_{i<j}^{N} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

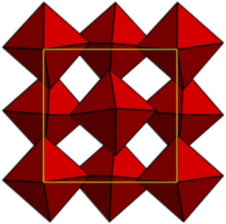
TABLE IV. Number of saddle points of each index for LJ_N clusters. The numbers in italics are likely to be far from complete.

	Stationary point index															
N	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
4	1	1	2	1	1	0	0									
5	1	2	4	6	6	2	1	0								
6	2	3	13	24	30	26	16	5	1	0						
7	4	12	44	98	168	190	168	101	45	11	1	0				
8	8	42	179	494	1000	1458	1619	1334	852	388	125	26	1	0		
9	21	165	867	2820	6729	12 093	16 292	16 578	13 226	8286	4053	1444	376	56	1	0
10	64	635	4074	16 407	46 277	*97 183*										
11	170	2424	17 109	*47 068*												
12	515	8607	*27 957*													
13	1509	28 756	*88 079*													

J. P. K. Doye and D. J. Wales, Saddle points and dynamics of Lennard-Jones clusters, solids, and supercooled liquids, The Journal of Chemical Physics, Vol. 116, pp. 3777–3788, 2002.

Use computational geometry, specifically close packings of convex/star convex sets, to find densest crystal structures or to remove from CSP those structures that are not packet closely together and thus speed up CSP and aid new crystal discovery.

CC3 is approximated by an octahedron



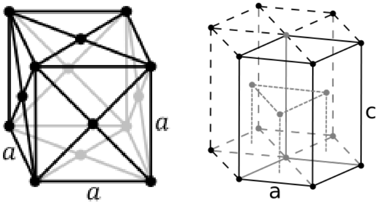
J. T. A. Jones et al., Modular and predictable assembly of porous organic molecular crystals, Nature vol. 474, p. 367–371, 2011.

How can one arrange most densely in space an infinite number of equal solids of given form, e.g. spheres with given radii or regular tetrahedra with given edges (or in prescribed position), that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as great as possible?

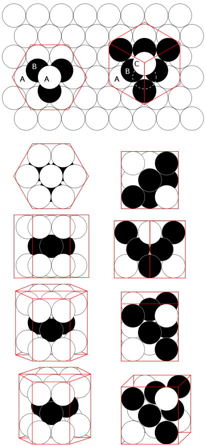
History

No packing of congruent balls in Euclidean three-space has density greater than that of the face-centered cubic packing (Johannes Kepler 1611).

FCC and HCP lattices

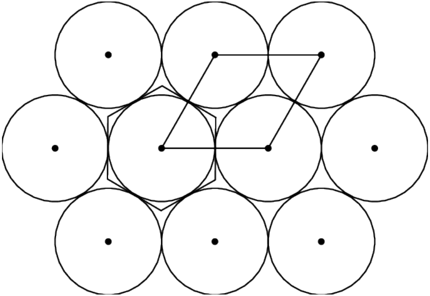


FCC and HCP lattice packings of spheres



- in 1831 Carl Friedrich Gauss proved to be true for lattice packings with density of $\frac{\pi}{3\sqrt{2}}$.
- in 2005 general proof of Thomas C. Hales was accepted to *Annals of mathematics.*

Regular hexagonal packing is the densest circle packing in the plane.



- in 1773 Joseph Louis Lagrange proved to be true for lattice packings with density of $\frac{\pi}{\sqrt{12}}$.
- in 1940 first rigorous proof by László Fejes Tóth for the general case.

Lattice packing

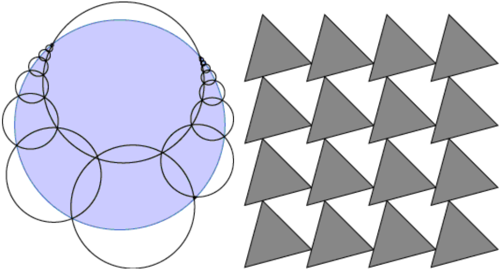
- **Covering:**
  the system of sets $S_1, S_2, \ldots$ is said to cover the set S, if

$$\bigcup_i S_i \supset S$$

- **Packing**
  the system of sets $S_1, S_2, \ldots$ is said to form a packing into the set S, if

$$S_i \cap S_j = \emptyset \ (i \neq j)$$
$$\bigcup_i S_i \subset S$$

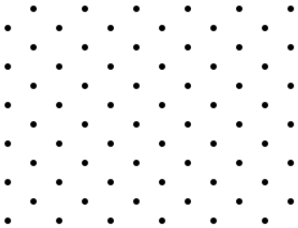
- $S = \mathbf{E}^n$
- $S_1, S_2, \dots$ is finite collection or countably infinite of translates and of a single compact convex set V. (Translate of V: set of all points of the form $\mathbf{v} + \mathbf{a}$, where $\mathbf{v} \in V$, and $\mathbf{a}$ is a fixed point or vector)



Let $\mathbf{a_1}, \mathbf{a_2}, \ldots, \mathbf{a_n}$ be n linearly independent vectors in $\mathbf{E}^n$,

$$\Lambda = \{u_1\mathbf{a_1} + u_2\mathbf{a_2} + \ldots + u_n\mathbf{a_n} \mid u_i \in \mathbb{Z}\}$$

is called a **lattice**.



$\mathcal{K}_L = \{V + \mathbf{b}_i \mid \mathbf{b}_i \in \Lambda\}$ - collection of translates of a set V

If V is a bounded set with positive measure and $\mathcal{K}_L$ is the collection of translates of V of a lattice Λ then we can define "**density**" $\mathcal{K}_L$

$$\rho(\mathcal{K}_L) = \frac{\mathrm{vol}(V)}{|\det(\Lambda)|}$$

where $\det(\Lambda)$ is the determinant of the generators of lattice Λ.

If $\mathcal{K}_L$ forms a *packing* then

$$\rho\left(\mathcal{K}_L\right) \leq 1$$

If $\mathcal{K}_L$ forms a *covering* then

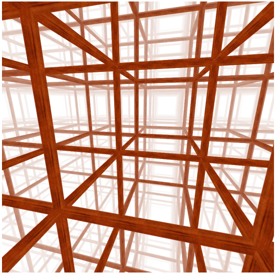
$$\rho\left(\mathcal{K}_L\right) \geq 1$$

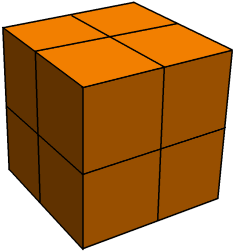
Example

Cubic honeycomb

When V is a cube we have a tiling and

$$\rho(\mathcal{K}_L) = 1$$





Example

What is the maximum packing density of balls in $\mathbf{E}^1$?

Bodies V for which maximum general packings are known

BODY	SOURCE
Circular disk in $\mathbb{E}^2$	[Thu10]
Parallel body of a rectangle	[Fej67]
Intersection of two congruent circular disks	[Fej71]
Centrally symmetric n-gon (algorithm in $O(n)$ time)	[MS90]
Ball in $\mathbb{E}^3$	[Hal05]
Ball in $\mathbb{E}^8$	[Via17]
Ball in $\mathbb{E}^{24}$	[CKM17]
Truncated rhombic dodecahedron in $\mathbb{E}^3$	[Bez94]

C. D. Toth, J. O'Rourke, J. E. Goodman eds., Handbook of Discrete and Computational Geometry 3rd Edition, CRC Press 2017.

d-dimensional balls for which maximum lattice packings are known

d	$\delta_L(B^d)$	SOURCE
2	$\frac{\pi}{2\sqrt{3}}$	[Lag73]
3	$\frac{\pi}{\sqrt{18}}$	[Gau]
4	$\frac{\pi^2}{16}$	[KZ72]
5	$\frac{\pi^2}{15\sqrt{2}}$	[KZ77]
6	$\frac{\pi^3}{48\sqrt{3}}$	[Bli35]
7	$\frac{\pi^3}{105}$	[Bli35]
8	$\frac{\pi^4}{384}$	[Bli35]
24	$\frac{\pi^{12}}{12!}$	[CK04]

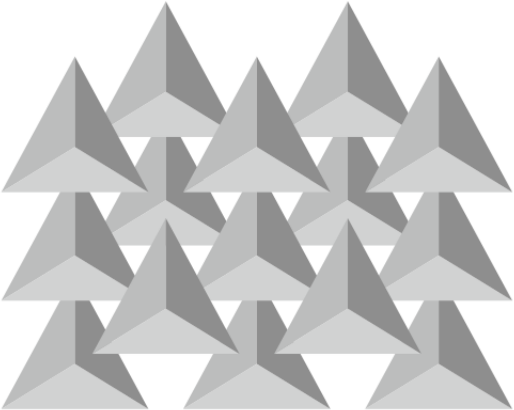
C. D. Toth, J. O'Rourke, J. E. Goodman eds., Handbook of Discrete and Computational Geometry 3rd Edition, CRC Press 2017.

Bodies V in $\mathbf{E}^3$ for which maximum lattice packings are known

BODY	$\delta_L(K)$	SOURCE
$\{x \mid \lvert x\rvert \le 1,\ \lvert x_3\rvert \le \lambda\} \quad (\lambda \le 1)$	$\pi(3-\lambda^2)^{1/2}/6$	[Cha50]
$\{x \mid \lvert x_i\rvert \le 1,\ \lvert x_1+x_2+x_3\rvert \le \lambda\}$	$\begin{cases} \frac{9-\lambda^2}{9} & \text{for } 0<\lambda\le\frac{1}{2} \\ \frac{9\lambda(9-\lambda^2)}{4(-\lambda^3-3\lambda^2+24\lambda-1)} & \text{for } \frac{1}{2}\le\lambda\le 1 \\ \frac{9(\lambda^3-9\lambda^2+27\lambda-3)}{8\lambda(\lambda^2-9\lambda+27)} & \text{for } 1\le\lambda\le 3 \end{cases}$	[Whi51]
$\{x \mid \sqrt{(x_1)^2+(x_2)^2}+\lvert x_3\rvert \le 1\}$	$\pi\sqrt{6}/9 = 0.8550332\ldots$	[Whi48]
Tetrahedron	$18/49 = 0.3673469\ldots$	[Hoy70]
Octahedron	$18/19 = 0.9473684\ldots$	[Min04]
Dodecahedron	$(5+\sqrt{5})/8 = 0.9045084\ldots$	[BH00]
Icosahedron	$0.8363574\ldots$	[BH00]
Cuboctahedron	$45/49 = 0.9183633\ldots$	[BH00]
Icosidodecahedron	$(45+17\sqrt{5})/96 = 0.8647203\ldots$	[BH00]
Rhombic Cuboctahedron	$(16\sqrt{2}-20)/3 = 0.8758056\ldots$	[BH00]
Rhombic Icosidodecahedron	$(768\sqrt{5}-1290)/531 = 0.8047084\ldots$	[BH00]
Truncated Cube	$9(5-3\sqrt{2})/7 = 0.9737476\ldots$	[BH00]
Truncated Dodecahedron	$(25+37\sqrt{5})/120 = 0.8977876\ldots$	[BH00]
Truncated Icosahedron	$0.78498777\ldots$	[BH00]
Truncated Cuboctahedron	$0.8493732\ldots$	[BH00]
Truncated Icosidodecahedron	$(19+10\sqrt{5})/50 = 0.8272135\ldots$	[BH00]
Truncated Tetrahedron	$207/304 = 0.6809210\ldots$	[BH00]
Snub Cube	$0.787699\ldots$	[BH00]
Snub Dodecahedron	$0.7886401\ldots$	[BH00]

C. D. Toth, J. O'Rourke, J. E. Goodman eds., Handbook of Discrete and Computational Geometry 3rd Edition, CRC Press 2017.

The densest lattice packing with the tetrahedron



I. Bárány,K. J. Böröczky, G. Fejes Tóth,J. Pach, J eds. Geometry - Intuitive, Discrete, and Convex—A Tribute to László Fejes Tóth. Berlin: Springer, 2014.

Minkowski sum

$$A + B = \{a + b : a \in A, b \in B\}$$

for sets A and B.

Difference body of A

$$D(A) = A + (-A)$$

for set A.

Packing lattice of a difference body

Example of difference bodies

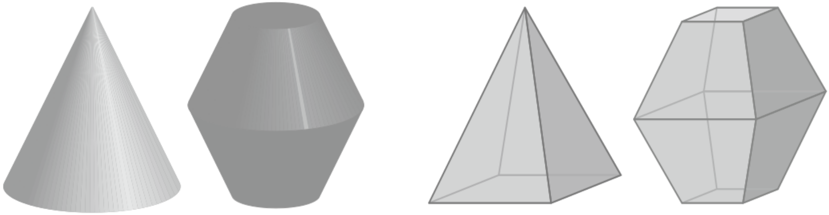


Fig. 5. Cones and their difference bodies: the circular cone and the square pyramid

I. Bárány,K. J. Böröczky, G. Fejes Tóth,J. Pach, J eds. Geometry - Intuitive, Discrete, and Convex—A Tribute to László Fejes Tóth. Berlin: Springer, 2014.

Lemma

Let a_1 and a_2 be two distinct points and let V be a convex set. Then $(V + a_1) \cap (V + a_2) \neq \emptyset$ if and only if

$$\left(\frac{1}{2}D(V) + a_1\right) \cap \left(\frac{1}{2}D(V) + a_2\right) \neq \emptyset.$$

From this lemma it follows that:

Λ is a packing lattice of $V \Leftrightarrow \Lambda$ is a packing lattice of $\frac{1}{2}D(V)$.

Appendix

Formal definition of packing and covering density, and supporting material for the simple proof of Thue's theorem.

$$\rho_{+}\left(\mathcal{K}, C\right) = \frac{1}{\mu\left(C\right)} \sum_{\left(V+\mathbf{a_i}\right)\cup C\neq\emptyset} \mu\left(V+\mathbf{a_i}\right)$$

$$\rho_{-}\left(\mathcal{K}, C\right) = \frac{1}{\mu\left(C\right)} \sum_{\left(V+\mathbf{a_i}\right)\subset C} \mu\left(V+\mathbf{a_i}\right)$$

- $\{\mathbf{a_i}\}$ - sequence of points
- $\mathcal{K} = \{V + \mathbf{a_i}\}$ - collection of translates of V
- C - cube with edge length s centred at some point $\mathbf{c}$
- $\mu\left(\cdot\right)$ - Lebesgue measure

Upper density

$$\rho_+(\mathcal{K}) = \limsup_{s(C)\to\infty} \rho_+(\mathcal{K}, C)$$

Lower density

$$\rho_-(\mathcal{K}) = \liminf_{s(C)\to\infty} \rho_-(\mathcal{K}, C)$$

Packing density of V

$$\delta(V) = \sup_{\mathcal{K}} \rho_+ (\mathcal{K})$$

supremum over all systems $\mathcal{K}$ of translates of V, which form packings into the whole space.

Covering density of V

$$\vartheta(V) = \inf_{\mathcal{K}} \rho_- (\mathcal{K})$$

infimum over all systems $\mathcal{K}$ of translates of V, which form a covering of the whole space.

Theorem

If V is bounded with a positive measure, its packing and covering densities satisfy

$$\delta(V) \leq 1 \leq \vartheta(V).$$

$\mathcal{K}_L = \{V + \mathbf{b}_i \mid \mathbf{b}_i \in \Lambda\}$ - system of translates of a set V

Lattice-packing density of V

$$\delta_L(V) = \sup_{\mathcal{K}_L} \rho_+ (\mathcal{K}_L)$$

$\mathcal{K}_L$ is a lattice-packing into the whole space.

$\mathcal{K}_P = \{V + \mathbf{c_j} + \mathbf{b}_i\}$

- $\mathbf{c_j} \in \mathbf{E}^n$ for $j = 1, \ldots, N$
- $\mathbf{b}_i$ - point of the lattice of all points that have integral multiples of a positive constant s for coordinates.
- s is the period of a periodic system $\mathcal{K}_P$.

Periodic packing density of V

$$\delta_P(V) = \sup_{\mathcal{K}_P} \rho_+ (\mathcal{K}_P)$$

$\mathcal{K}_P$ is a periodic packing into the whole space.

Theorem

Let V be a bounded set with a positive measure. Let $\mathbf{T}$ be a non-singular affine transformation. Then

$$\delta\left(\mathbf{T}V\right) = \delta_P\left(V\right) = \delta\left(V\right),$$
$$\delta_L\left(\mathbf{T}V\right) = \delta_L\left(V\right).$$

Lattice packings

Theorem

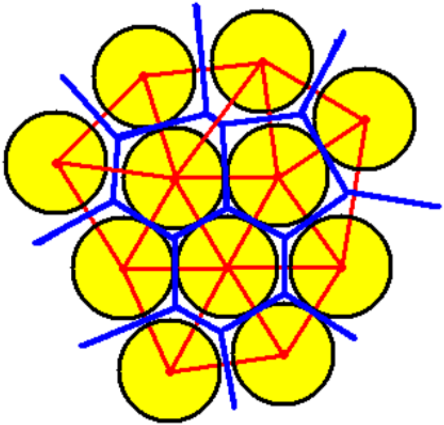
Let V be a bounded set with positive measure. Let $\mathcal{K}_L$ be the system of translates of V of a lattice Λ. Then

$$\rho_+(\mathcal{K}_L) = \rho_-(\mathcal{K}_L) = \frac{\mu(V)}{|\det(\Lambda)|}$$

where $\det(\Lambda)$ is the determinant of the generators of lattice Λ.

On the simple proof of Thue's theorem

Delunay triangulation of a circle configuration



On the simple proof of Thue's theorem