Sphere packings, crystals, and error-correcting codes

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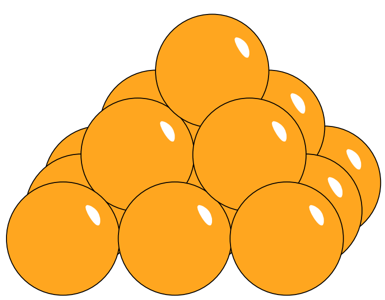
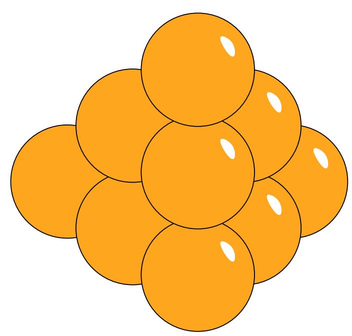
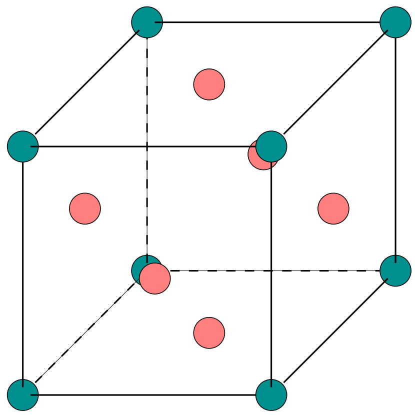
What is the densest packing?



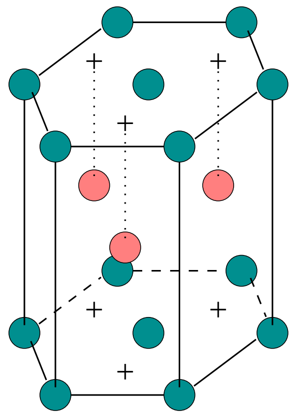


Atoms in crystals

The two densest packings:

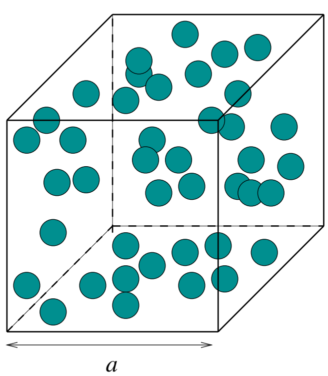


"face-centered cubic"



"hexagonal close packing"

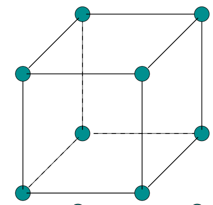
Mathematical definition of density



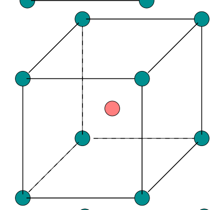
$$\delta = \lim_{a \to +\infty} \frac{\text{volume of balls}}{\text{volume of cube}}$$

Examples:

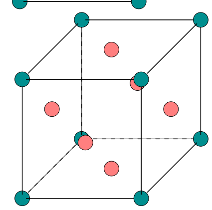
simple cubic: $\delta = \frac{\pi}{6} \simeq 0.5236$

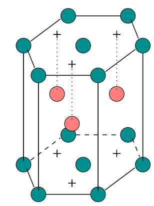


centered cubic: $\delta = \frac{\pi\sqrt{3}}{8} \simeq 0.6802$



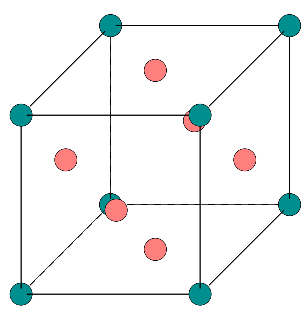
$$\left.\begin{array}{r}\text{face-centered cubic}\\ \text{hexagonal close}\end{array}\right\} \quad \delta = \frac{\pi}{3\sqrt{2}} \simeq 0.7405$$



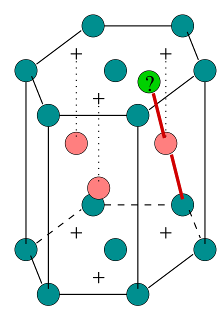


Various packing problems

- ▷ in any dimension
- ▷ finite packing (completely open)
- ▷ for **lattices**
  (translation invariance)



lattice



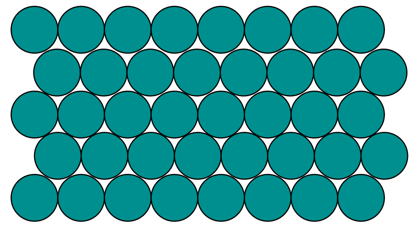
not a lattice

Kepler's conjecture (1610)

Maximal density of a sphere packing in 3-space is $\frac{\pi}{3\sqrt{2}} \simeq 0.7405$
(= face-centered cubic lattice)

Proved by Thomas Hales in 1998.

In the plane: optimal density is $\frac{\pi}{2\sqrt{3}} \simeq 0.9069$
(proved by Thue, 1892, 1910)



In dimensions $4, 5, 6, 7, 8$, densest *lattices* are known. Best known packings are often lattices, but not always (e.g. dims. 10, 11, 13).

(Reference: N.J.A. Sloane, *The sphere packing problem*,
http://www.math.uiuc.edu/documenta/xvol-icm/13/Sloane.MAN.ps.gz)

Various 3D conjectures

- Kepler conjecture (Hales 1998):
  Max. density of a sphere packing $= \frac{\pi}{3\sqrt{2}} \simeq 0.7405$.
- Kissing number conj. (Newton) (van der Waerden–Schütte 1953; Leech 1956):
  A sphere can be in contact with at most 12 other spheres.
- Dodecahedral conjecture (Fejes Tóth 1942) (Hales-McLaughlin 1998):
  Volume of Voronoi cell $\geq$ regular dodecahedron ($\Rightarrow$ packing density ≤ 0.755).

Hales' proof of Kepler uses:
$\triangleright$ Fejes Tóth: reduce to optimization problem in finitely many variables
(local configurations – Fejes Tóth: weighted averages of adjacent Voronoi cells)
$\triangleright$ Computer calculations (to classify local configurations; to solve optimization problem)

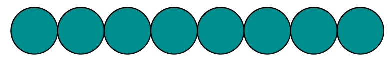
(Reference: T. Hales, *An overview of the Kepler conjecture*, http://arxiv.org/abs/math.MG/9811071)

Laminated lattices

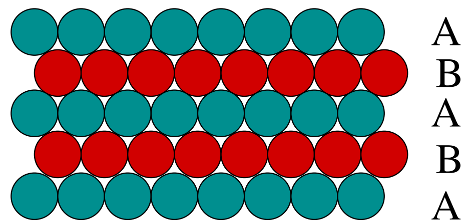
Stack layers of $(n-1)$-dimensional lattices (in "deepest holes")

Laminated lattices are the densest ones up to dimension 8.

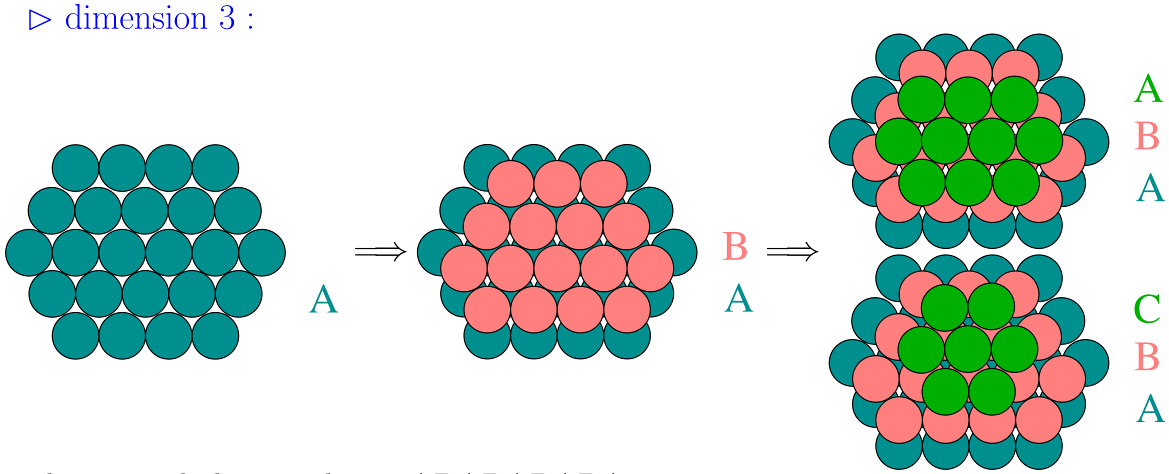
▷ dimension 1



▷ dimension 2

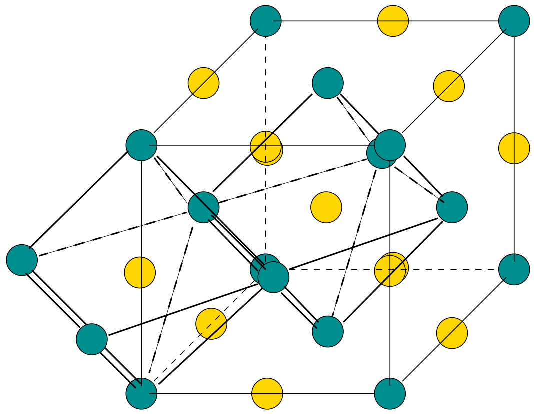


▷ dimension 3 :



hexagonal close packing: ABABABABA...
face-centered cubic: ABCABCABC... (only lattice)
irregular packings: e.g. ABABCACBA...

▷ dimension 4:



"octahedral sites"
(natural location of doping atoms in *f.c.c.* crystals)

1st layer:

(0,0,0,0)	(0,1,1,0)	(1,0,1,0)	(1,1,0,0)
(2,0,0,0)	(2,1,1,0)	(3,0,1,0)	(3,1,0,0)
(0,2,0,0)	(0,3,1,0)	(1,2,1,0)	(1,3,0,0)
(0,0,2,0)	(0,1,3,0)	(1,0,3,0)	(1,1,2,0)
...			

2nd layer:

(1,0,0,1)	(0,1,0,1)	(0,0,1,1)	(1,1,1,1)
(3,0,0,1)	(2,1,0,1)	(2,0,1,1)	(3,1,1,1)
(1,2,0,1)	(0,3,0,1)	(0,2,1,1)	(1,3,1,1)
(1,0,2,1)	(0,1,2,1)	(0,0,3,1)	(1,1,3,1)
...			

3rd layer = 1st layer + (0,0,0,2)

Coding theory

(N, n, k)-code: choose 2^n binary words of length N ($\{0,1\}^n \hookrightarrow \{0,1\}^N$) so that Hamming distance between valid code words is $\geq k$.

($\Rightarrow$ can detect and correct $[\frac{k-1}{2}]$ errors).

(Applications: data storage / communications ...)

Periodization $\Longrightarrow$ codes can be a source of dense sphere packings (& vice-versa).

(though most commonly used codes = polynomial interpolation / finite fields)

Examples:

▷ dimension 3, f.c.c. lattice is a (3,2,2)-code: 000,011,101,110
(3 bits = 2 data bits + 1 bit to detect a single error)

▷ dimension 4, densest lattice is a (4,3,2)-code:
0000,0011,0101,0110,1001,1010,1100,1111
(4 bits = 3 data bits + 1 bit to detect a single error)

▷ dimension 7: (7,4,3) "perfect Hamming code":
0000000, 0001110, 0010101, 0011011, 0100011, 0101101, 0110110, 0111000,
1000111, 1001001, 1010010, 1011100, 1100100, 1101010, 1110001, 1111111
(7 bits = 4 data bits + 3 bits to correct a single error)

▷ dimension 24: Leech lattice ($=\Lambda_{24}$): the densest known packing in dim. 24.
(and in nearby dimensions, by taking sections or stacking layers).
It has the highest possible kissing number (each sphere touches 196560 others!)
It is a laminated lattice but can also be constructed from a (24,12,8)-code.

Bibliography:

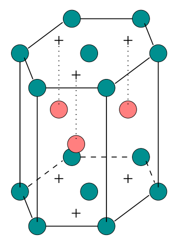
- N.J.A. Sloane, *The sphere packing problem*,
  http://www.math.uiuc.edu/documenta/xvol-icm/13/Sloane.MAN.ps.gz
- J.H. Conway, N.J.A. Sloane, *Sphere packings, lattices and groups*,
  Springer-Verlag, 3rd edition, 1998.
- T. Hales, *An overview of the Kepler conjecture*,
  http://arxiv.org/abs/math.MG/9811071
- G. Szpiro, *Kepler's conjecture: How some of the greatest minds in history helped solve one of the oldest math problems in the world*, John Wiley & Sons, 2003

HOMEWORK

Problem 1.

The purpose of this problem is to verify that the density of the hexagonal close packing is equal to that of the face-centered cubic lattice ($\delta = \frac{\pi}{3\sqrt{2}}$).

Consider the hexagonal close packing with spheres of radius r:



a) Express in terms of r the distance h (in the "vertical" direction) between two consecutive layers of spheres. (Recall that inside each layer the spheres are in contact with each other, and that the successive layers rest on top of each other).

b) Use your result to find the volume of the prism with hexagonal base and height $2h$ shown in the picture; deduce the density of the hexagonal close packing.

Problem 2.

The goal of this problem is to find the density of the laminated lattice packing in 4-dimensional space (see slide # 10).

a) The 4-dimensional ball of radius a centered at the origin is the set of all points (x, y, z, u) whose distance to the origin $d = \sqrt{x^2 + y^2 + z^2 + u^2}$ is less than a. Similarly to the familiar case of the 3-ball, its volume V is given by the iterated integral

$$\iiiint dV = \int_{-a}^{a} \int_{-\sqrt{a^2-x^2}}^{\sqrt{a^2-x^2}} \int_{-\sqrt{a^2-x^2-y^2}}^{\sqrt{a^2-x^2-y^2}} \int_{-\sqrt{a^2-x^2-y^2-z^2}}^{\sqrt{a^2-x^2-y^2-z^2}} du\, dz\, dy\, dx,$$

Prove (by evaluating the integral) that $V = \frac{1}{2}\pi^2 a^4$.

(Hint: switch to 3D spherical coordinates after evaluating the inner-most integral! You will eventually obtain a single integral which can be evaluated by making the change of variables $\rho = \sin t$.)

b) Consider the laminated packing of 4-space: how many balls are contained in the 4-cube of side 2 whose projection is represented on slide # 10 ? Count those balls which cross the boundary with a fractional coefficient according to how much of the ball lies within the cube. (The cube is given by $0 \le x \le 2$, $0 \le y \le 2$, $0 \le z \le 2$, $0 \le u \le 2$.)

Remark: although balls are counted with fractional coefficients, your final answer will be an integer. Optional: explain a more efficient way of obtaining this answer.

c) Show that the density of this packing is $\simeq 0.617$. (Find an exact formula.)

(Note: the radius of the balls is **not** equal to 1; otherwise the balls centered at $(0, 0, 0, 0)$ and $(1, 1, 0, 0)$ would interpenetrate!)