Problems with packing periodicity

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Zahlentheoretisches Kolloquium
December 11, 2015

Abstract

When we think about packing problems, our intuition often leads us to believe that the solutions should exhibit some exceptional symmetry. I'll survey some interesting problems and examples dealing with packing and periodicity, particularly some that break more symmetry than you might think.

In this context, I'll also tell you about recent joint work on packings of a generic polygon in the plane: By introducing a useful topology on packings and describing the local optimality of a configuration among double lattices as a consequence of an algorithm of Mount, linear programming techniques can often certify the best double lattice packing as a local maximum for volume fraction among all packings.

Packing Problems

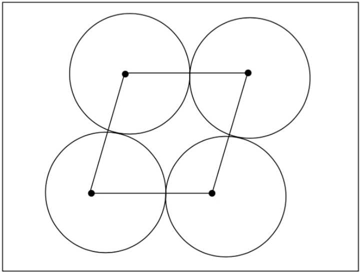
Given $\mathcal{K}$, a collection of congruent objects K in $\mathbb{R}^n$, it forms a *packing* if no K overlap.

The density $\rho(\mathcal{K})$ of a packing $\mathcal{K}$ is the asymptotic volume fraction

$$\rho(\mathcal{K}) = \limsup_{r\to\infty} \frac{\mathrm{Vol}(\mathcal{K} \cap B^n(r))}{\mathrm{Vol}(B^n(r))}.$$

For an object K, the maximum density over all packings $\mathcal{K}$ in the class of lattices, translations and packings are $\rho_L(K)$, $\rho_T(K)$, $\rho(K)$.

In the context of p. d. quadratic forms, Lagrange (1773) and Gauss (1831) showed the hexagonal circle packing and the FCC lattice were the best in two and three dimensions.



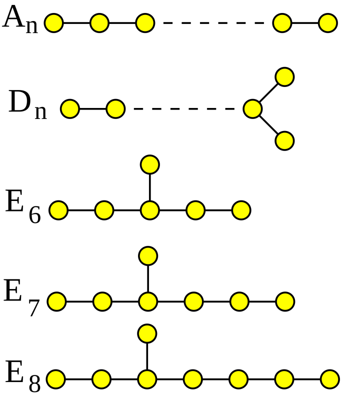
Given a lattice packing in $\mathbb{R}^2$, force two circles to touch. This gives a strand of circles. These strands may also be forced to touch. Locally, we find configurations of parallelograms.

Best Lattice Packings

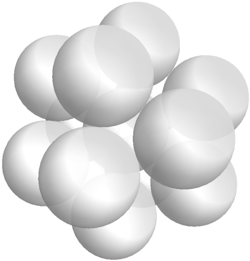
In low dimensions, the best lattice sphere packings are described by simply laced root systems: A_1, A_2, A_3, D_4, D_5, E_6, E_7, E_8.

In $\mathbb{R}^2$, it is known that the lattice packing is the best packing for all convex, 0-symmetric bodies.

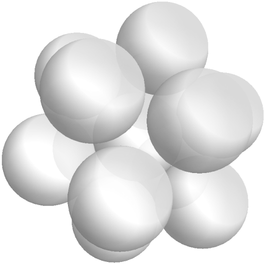
The densest sphere packing in $\mathbb{R}^3$ is attained by A_3, but it is not unique. By $\mathbb{R}^{10}$, the best packing known is not a lattice packing; rather it comes from a special binary code.



Local Spheres



FCC



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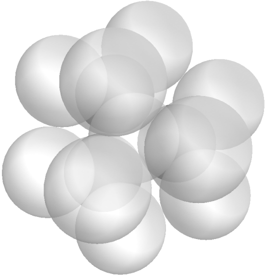


HCP

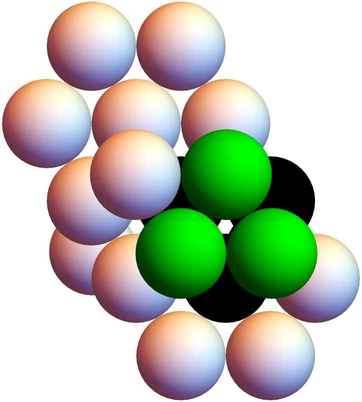
Improving Packing Density

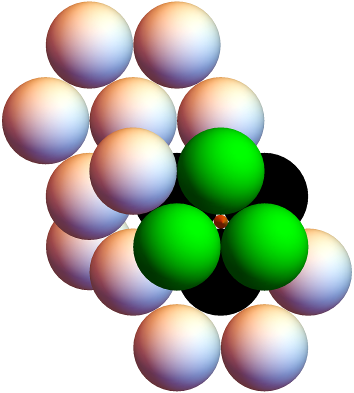
Consider a packing by unit radius balls in $\mathbb{R}^3$ that achieves the maximum density of $\pi/\sqrt{18}$, the density of the FCC packing.

Notice that the HCP packing has the same density, and it also will has holes all the way through it. We can thread ellipsoids with minor radii a and major radius b chosen to have the same volume as the spheres through those holes.

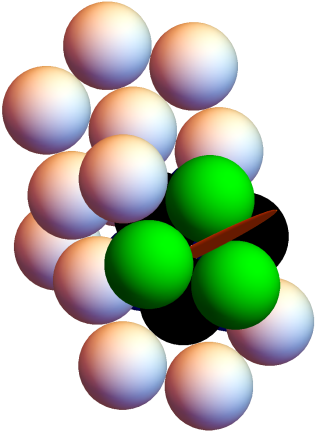
Remark

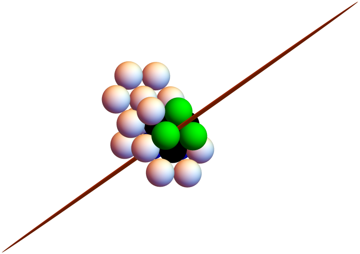
$$V = \frac{4}{3}\pi aab$$





Improving Packing Density





Improving Packing Density

Then we can apply the linear transformation

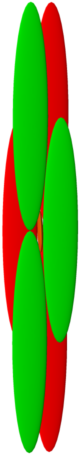
$$\begin{pmatrix} a^2b & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a^2 \end{pmatrix},$$

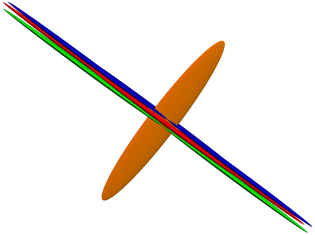
taking $\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$ & $\begin{pmatrix} a \\ a \\ b \end{pmatrix}$ to $\begin{pmatrix} 1 \\ a \\ a^2 \end{pmatrix}$ & $\begin{pmatrix} a \\ a^2 \\ 1 \end{pmatrix}$ respectively.

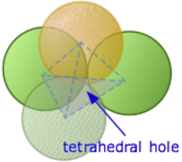
Remark

This transformation scales the volume but preserves density.

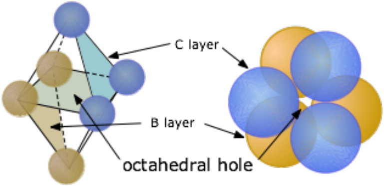
Improving Packing Density







Lattice packings of spheres can have ”deep wells”. This is useful for finding exceptionally dense lattices in certain dimensions. Provided they are large enough, the deep wells can be used to add additional spheres.



Heuristics

When wells are not deep enough and spheres cannot be added, bulk symmetry seems to conflict with high density. Using a coarse heuristic – lattices are only quadratically specified in the dimension – there is room in high dimensions.

Question (Rogers)

- *Is it true that dense lattice packings of spheres are dense?*

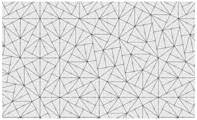
Conjecture (Torquato)

- *Dense sphere packings are disordered in high dimensions.*

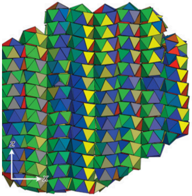
Question

Are there other structures that force aperiodicity in the bulk?

Aperiodic tilings.



High density polytopes.



Barlow packings, counterexamples to the Keller conjecture...

I have given you some problems and promised some results. Let me describe some recent work on the local density of packings with Yoav Kallus and a program to address global density with Tom Hales, related to the two following conjectures.

Conjecture (Almost Certainly False)

The densest packing of pentagons is aperiodic.

Conjecture (Almost Certainly True)

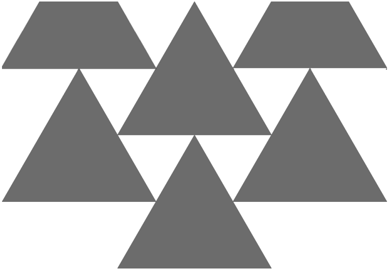
The densest packing of pentagons is a double lattice.

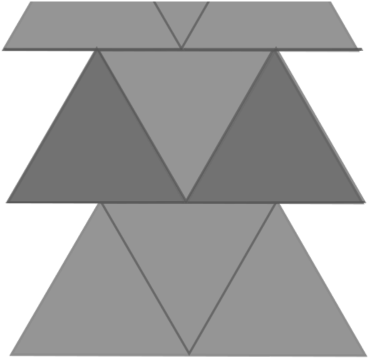
The best packing of pentagons is probably not aperiodic, it is probably a double lattice packing with density $0.9213\ldots$

Double Lattices

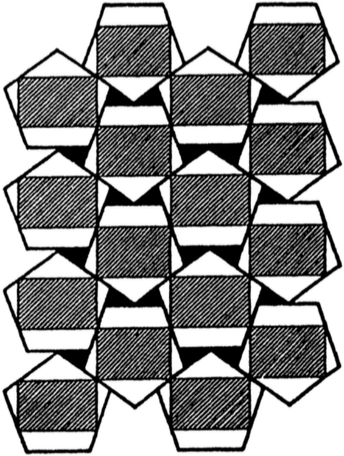
Remark

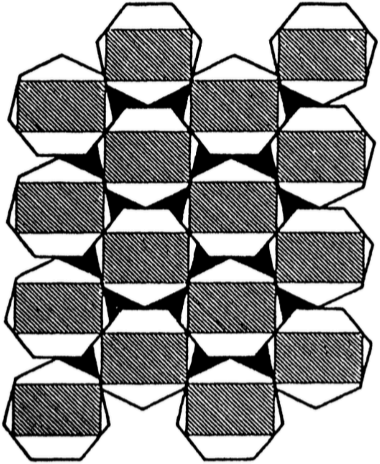
With triangles we can certainly break symmetry and do better!





Double Lattices





Topologies on Packing Space

Since we are considering a maximal density problem, we can restrict to the collection of saturated packings; those to which we cannot add another object. Nice topologies come from:

- The Hausdorff metric with the full packing considered as a subset.
- A finite ball metric, localizing the Hausdorff metric to a large ball.

These do not correspond to our idea of a "nearby packing." In the Hausdorff topology, rescaling is is a discontinuous motion. The finite ball topology is too coarse to discuss local optimality of density. It does not detect arbitrary rearrangement.

Definition

Let Ξ be a set of isometries. Ξ is a (r, R)-set if the point set $\{\xi(0) : \xi \in \Xi\}$ has packing radius $> r$ and covering radius $< R$.

Definition

Given two (r', R')-sets Ξ and Ξ' of isometries, we define the premetric

$$\delta_R(\Xi, \Xi') = \inf_{\text{enum.}} \sup\{||\xi_i^{-1}\xi_j - \xi_i'^{-1}\xi_j'|| :$$

$$i, j \text{ such that } ||\xi_i(0) - \xi_j(0)|| < 2R \text{ or } ||\xi_i'(0) - \xi_j'(0)|| < 2R\}.$$

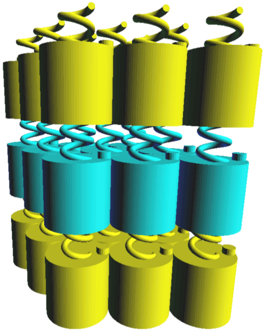
The infimum is over all enumerations $\mathbb{N} \to \Xi$ and $\mathbb{N} \to \Xi'$.

Raft Topology

This combines the Hausdorff and finite ball topologies.

For a fixed enumeration, the ξ_i^{-1} send points to a neighborhood of 0, and the norm considers the maximum perturbation inside a ball of radius R for all such balls about points. This is then minimized over all global identifications.

This is like a raft, tied together with strings of length $< R$.



Remark

Discontinuous motions!

Definition

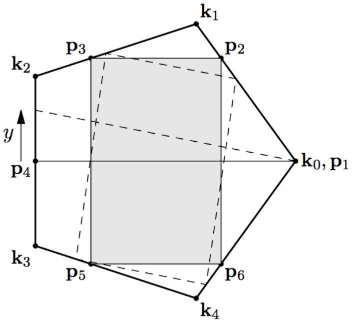
A chord of a convex body K is a line segment whose endpoints lie on the boundary of K. A chord is an affine diameter if there is no longer chord parallel to it.

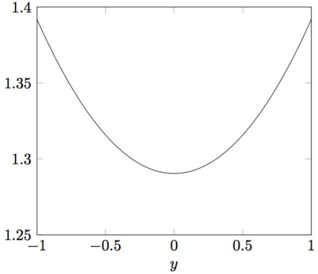
Definition

The convex hull of two parallel chords that are half the length of the parallel affine diameter is called a half-length parallelogram.

An affine diameter of K might not not uniquely determine the half-length parallelogram (consider for example a square), but it does uniquely determine the area.

Double Lattices





Double Lattices

Definition

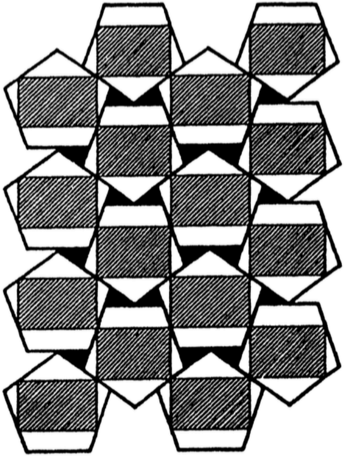
A set $\Lambda \subset E(n)$ is called a (full rank) double lattice if it is an (r, R)-set for some $r > 0$ and $R < \infty$, it consists of translations and point reflections, it is closed under composition and inversion, and it is not a lattice (that is, includes at least one point reflection).

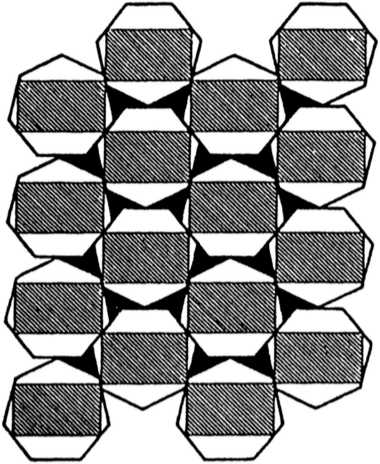
An n-dimensional double lattice is generated by a lattice and a point reflection, or alternatively by reflections about $n + 1$ affine-independent points or by reflections about the $2n$ vertices of a parallelepiped.

Theorem (Kuperberg and Kuperberg, Mount)

For a planar convex body K, an double lattice packing of highest density is generated by reflection about the vertices of a half-length parallelogram.

Double Lattices





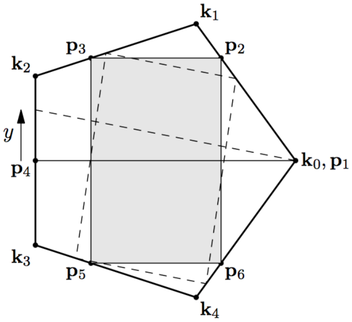
Mount Algorithm

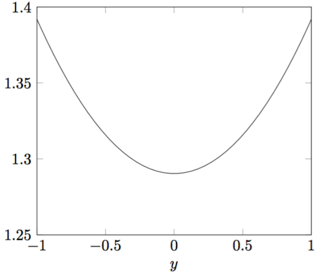
The affine diameter of a convex polygon is well behaved but with some non-trivial considerations as the diameter rotates. The behavior of the vertices of the half-length parallelogram are described by an *interspersing property*; they are non-decreasing functions in the rotation of the affine diameter.

Proposition (Initialization)

there is an affine diameter of a convex polygon K in every direction that meets a vertex.

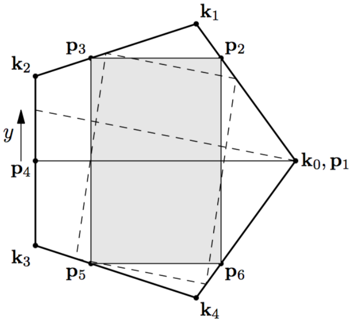
Given an initial affine diameter in a particular direction, the affine diameter can be tracked by sweeping out the ray in a clockwise direction from the initial vertex until it meets another vertex. From there, it is possible that the affine diameter continues to extend from the original vertex or that it begins to sweep out clockwise from the opposite vertex.

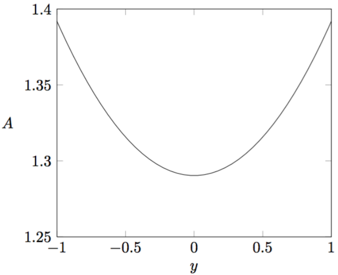

k1
p3
p2
k2
y
p4
k0, p1
k3
p5
p6
k4


1.4
1.35
1.3
1.25
A
−1
−0.5
0
0.5
1
y

In order to generate the densest double lattice packing, find the minimal area half-length parallelogram. This is done by moving between *critical angles* of the affine diameter: those angles where a vertex of the half-length parallelogram or both vertices of the affine diameter meet vertices of K. It is possible to tracking the motion via a parametrization of the slopes along which the vertices must travel between certain critical angles where the the area function becomes non-analytic. This is exactly where the moving end of the affine diameter or a vertex of the half length parallelogram meet a vertex of K. Note that these also correspond to the degenerate situations.

Double Lattices





Away from those critical angles, we have the following:

$$\mathbf{p}_i(t) = \mathbf{p}_i^{inital} + \alpha_i t \mathbf{v}_i$$

satisfying

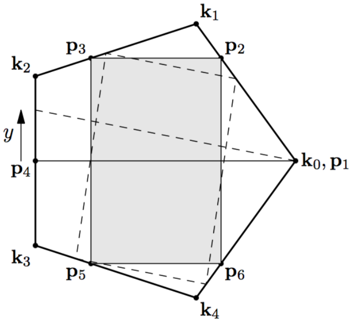
$$\frac{\mathbf{p}_4(t) - \mathbf{p}_1}{2} = \mathbf{p}_3(t) - \mathbf{p}_2(t)$$

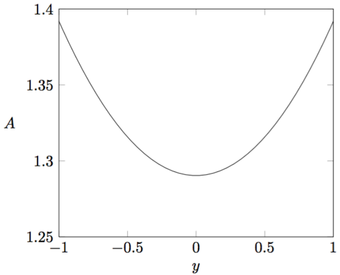
and

$$\frac{\mathbf{p}_4(t) - \mathbf{p}_1}{2} = \mathbf{p}_5(t) - \mathbf{p}_6(t)$$

This system can be solved for the rate constants α_i which give conditions on the motion of the parallelogram. We fix the affine diameter as a horizontal chord of length one, define variable motions of the point $\mathbf{p}_i$ at inclination ϕ_i and let the moving end of the affine diameter move at unit speed.

Mount Algorithm





Solving this system yields rate constants

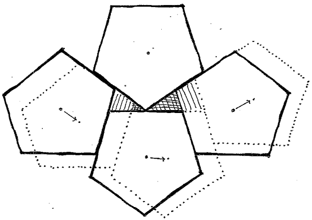
$$\begin{aligned}
\alpha_1 &= 0 \\
\alpha_2 &= \frac{\sin\left(\phi_3 - \phi_4\right)}{2\sin\left(\phi_2 - \phi_3\right)} \\
\alpha_3 &= \frac{\sin\left(\phi_2 - \phi_4\right)}{2\sin\left(\phi_2 - \phi_3\right)} \\
\alpha_4 &= 1 \\
\alpha_5 &= \frac{\sin\left(\phi_4 - \phi_6\right)}{2\sin\left(\phi_5 - \phi_6\right)} \\
\alpha_6 &= \frac{\sin\left(\phi_4 - \phi_5\right)}{2\sin\left(\phi_5 - \phi_6\right)}
\end{aligned}$$

The minimum value of the area between critical angles is determined completely by the data at the critical angles.

Non-lattice Packings

Mount gives us an algorithm to find and characterize the best double lattice for polygons. How do we extend this to a general packing?

Consider the previously introduced raft topology. It is particularly nice with respect to double lattices and allows us to consider minimizing the volume of two Delone triangles in packings of four objects, a nonlinear optimization problem in 9 variables.



LP Theorem

Consider the nonlinear optimization problem

$$\begin{aligned} \text{minimize } & f(x), \\ \text{over } & x \in \mathbb{R}^n, \\ \text{subject to } & g_r(x) \geq 0, r \in I, \\ & \|x\| \leq \epsilon. \end{aligned}$$

We can show that the following conditions are sufficient for the origin to be the unique solution of this system for some $\epsilon > 0$.

Let e_1 denote the standard unit vector $(1, 0, \ldots, 0) \in \mathbb{R}^n$, $E = \{te_1\}$ its span, and H the orthogonal complement, so that $\mathbb{R}^n = E \oplus H$.

LP Theorem

Conditions

- *I is a finite set.*
- *$f(x)$ and $g_r(x)$, $r \in I$, are continuously differentiable. Denote $F(t) = \nabla f(te_1)$ and $G_r(t) = \nabla g_r(te_1)$.*
- *$f(0) = g_r(0) = 0$ for all r in I.*
- *The linear program*

  $$\text{minimize}_{x\in\mathbb{R}^n} F(0)\cdot x \ \ subject\ to\ G_r(0)\cdot x \geq 0, r \in I$$

  has E as the set of solutions.

Conditions (continued)

- *There is an $\epsilon > 0$ so the functions $g_r(te_1) = 0$ for all $-\epsilon < t < \epsilon$, $r \in I$.*
- *$f(te_1)$ has an isolated local minimum at $t = 0$.*

Theorem

Given the conditions, there exists $\epsilon > 0$ such that the origin is the unique solution of

$$\begin{aligned} \text{minimize } & f(x), \\ \text{over } & x \in \mathbb{R}^n, \\ \text{subject to } & g_r(x) \geq 0, r \in I, \\ & \|x\| \leq \epsilon. \end{aligned}$$

.

Local Optimality For General Polygons

Pentagons are the easiest case locally, as the density and mean volume functions both satisfy this theorem directly.

In general, we need to add an auxiliary function to the mean volume that only acts locally, swapping volume symmetrically with the nearest neighbors. This may be chosen as a linear combination of area swaps across the boundaries of the fundamental domain, weighted that the objective falls inside the dual cone of the constraints. The existence of such weights can be explicitly constructed for various small examples, and in general derived from the stability conditions that characterize the minimal half-length parallelogram.

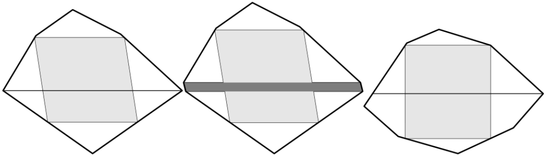
Remark

The cone condition can shown using interval arithmetic, or symbolically over an extension field.

Exceptions: Rare or Perturbable

Definition

- If $\mathbf{p}_2$ and $\mathbf{p}_6$ are in the interiors of edges that meet at $\mathbf{p}_1$ and $\mathbf{p}_3$ and $\mathbf{p}_5$ are in the interiors of edges that meet at $\mathbf{p}_4$.
- If the affine diameter parallel to $\mathbf{p}_2\mathbf{p}_3$ is not unique, then if $\mathbf{p}_2$ and $\mathbf{p}_3$ are in the interior of edges that have as endpoints the endpoints of one such affine diameter and $\mathbf{p}_5$ and $\mathbf{p}_6$ are in the interior of edges that have as endpoints the endpoints of another such affine diameter.
- If $\mathbf{p}_3$ and $\mathbf{p}_4$ are in the interior of the same edge, and $\mathbf{p}_2$ is at a vertex.



Theorem

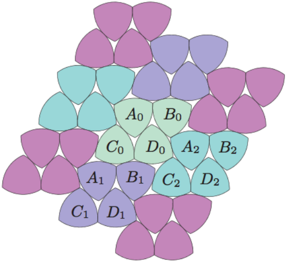
Any double-lattice packing that is an isolated local minimum among double-lattice packings and is not one of the exceptional types is a local minimum in the raft topology.

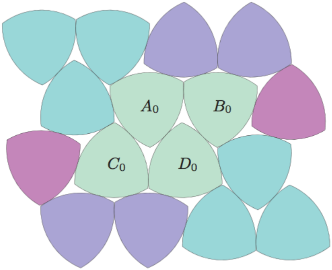
In practice, we have a procedure which, when combined with the Mount algorithm, takes a general polygon as input, produces the densest double lattice packing, and certifies it as local maximum among general packings.

If the densest double lattice packing is not an isolated maximum or is of exceptional type, further analysis is necessary.

Question

What happens with non-polygons?





Comment On Global Pentagons

Extending the local analysis of clusters of four is an optimization problem in a compact setting, since saturation gives a bound on the Delone triangles. This may be enough to solve the global pentagon problem, given enough case-by-case analysis.

This program consists of classifying configuration types and finding good local parameterizations for different types of configurations. The domain can then be meshed with respect to this atlas and the density locally bounded.

It is still being implemented, but looks promising. So far we have reduced the global density bound for pentagons from 0.981 to 0.961 and the sharp result seems to follow from some reasonable conjectures.

Y. Kallus and W. Kusner, *The local optimality of the double lattice packing.* arXiv preprint arXiv:1509.02241.

wkusner.github.io

Supported by Austrian Science Fund (FWF) Project 5503 and National Science Foundation (NSF) Grant No. 1104102.

Bonus Question

Unlike the case for spheres, we have an example where

$$\rho_L(K) < \rho(K).$$

A similar construction for ellipses gives an example where

$$\rho(A) \times \rho(B) < \rho(A \times B).$$

Question

$$\rho_L(A \times B) \stackrel{?}{=} \rho_L(A) \times \rho_L(B)$$

$$\rho_T(A \times B) \stackrel{?}{=} \rho_T(A) \times \rho_T(B)$$