Do non-spheres always pack more densely than spheres?

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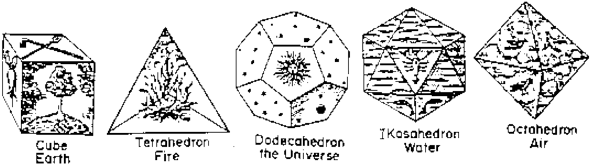
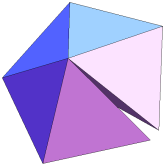
Santa Fe Institute

International Workshop on Jamming and Granular Matter
Queen Mary University of London
July 14, 2016

The long history of packing problems

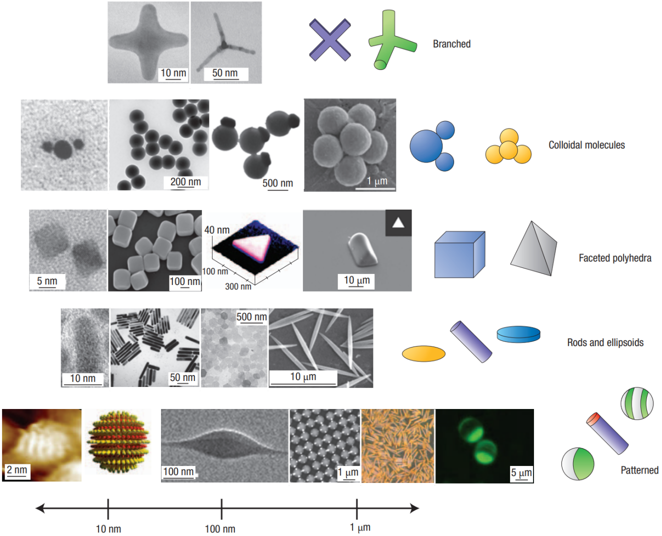




"In general, the attempt to give a shape to each of the simple bodies is unsound, for the reason, first, that they will not succeed in filling the whole. It is agreed that there are only three plane figures which can fill a space, the triangle, the square, and the hexagon, and only two solids, the pyramid [tetrahedron] and the cube."

– Aristotle. *On the Heavens*, volume III

Building blocks by design



Glotzer and Solomon, Nature Materials 2007

Packing problems in the modern era

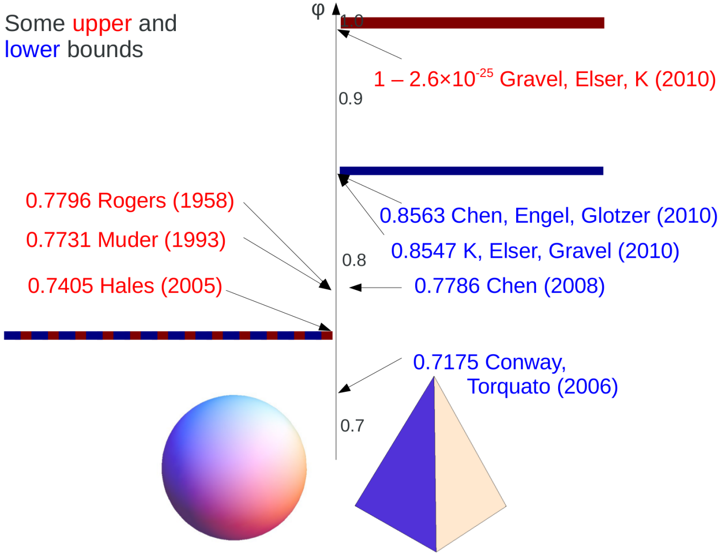
"How can one arrange most densely in space an infinite number of equal solids of a given form, e.g., **spheres** with given radii or regular **tetrahedra** with given edges, that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as large as possible?"

Theorem (Hales)

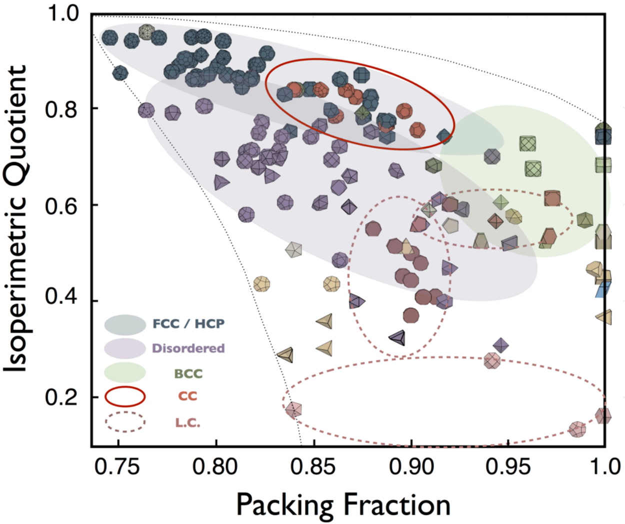
No sphere packing fills more than 0.7404 *of space.*

Figures for which optimal packing density is known: space filling tiles, 2D 2-fold-symmetric shapes, 3D spheres (and corollaries).

Packing regular tetrahedra

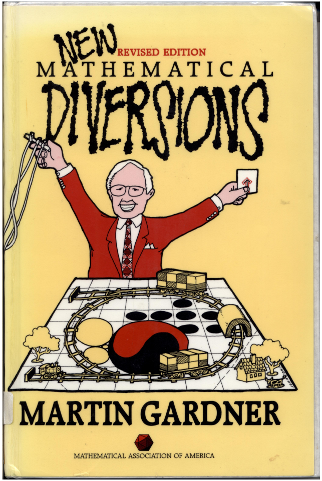


Packing convex shapes



Damasceno, Engel, and Glotzer, 2012.

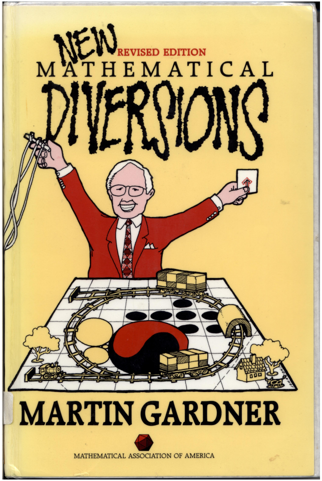
Ulam's Conjecture



"Stanislaw Ulam told me in 1972 that he suspected the sphere was the worst case of dense packing of identical convex solids, but that this would be difficult to prove."

1995 postscript to the column "Packing Spheres"

Ulam's Last Conjecture



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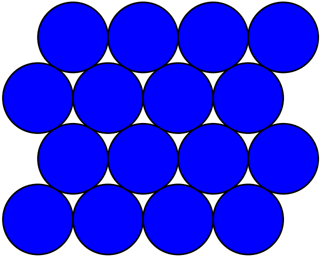
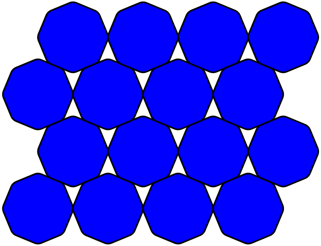
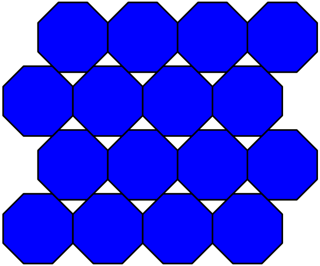
In 2D disks are not worst



$\phi = 0.9069$

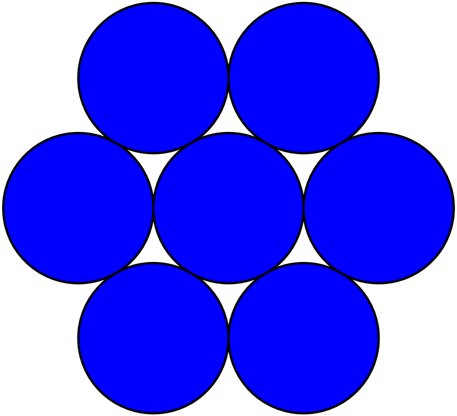


$\phi = 0.9024$



$\phi = 0.9062$

Why can we improve over circles?



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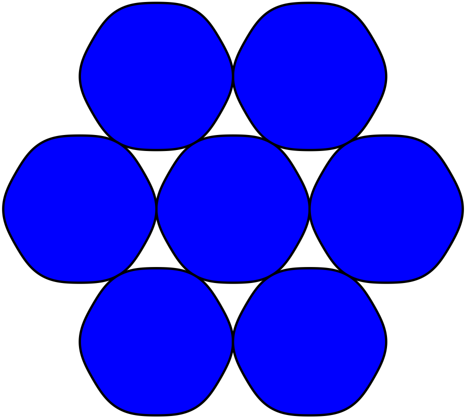

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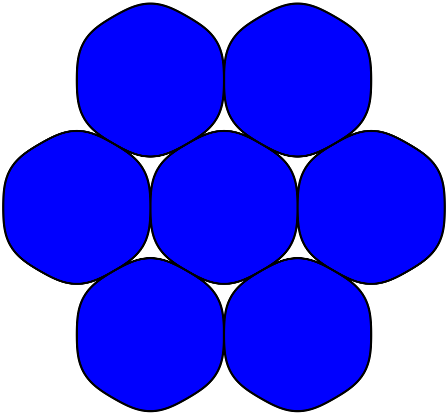

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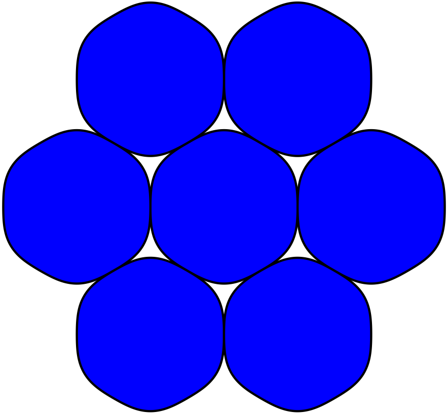


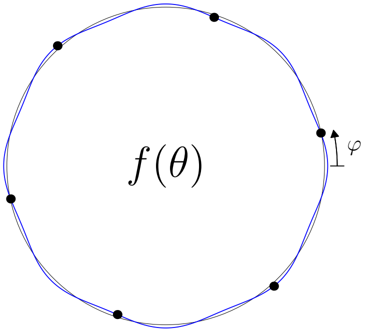
To first order:

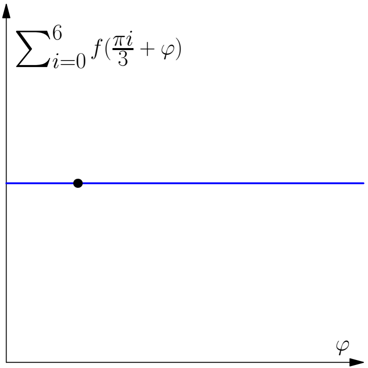
Δ(vol. per particle) $\propto$ average of deformation in the contact dirs.

Δ(vol. of particle) $\propto$ average of deformation in all dirs.

So, we can only hope to break even, and make up in higher orders.

Why can we improve over circles?





$$f(\theta) = 1 + \epsilon cos(8\theta)$$

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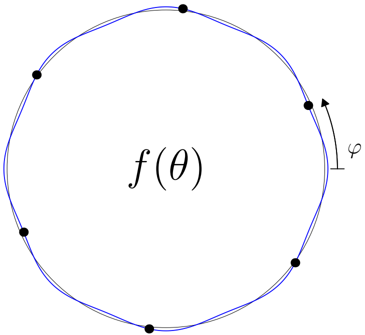

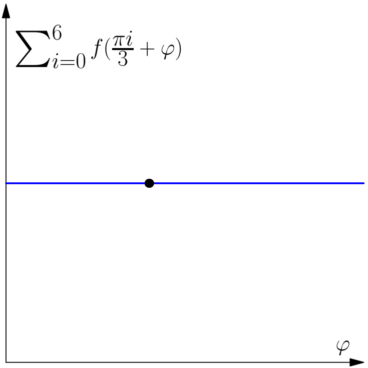

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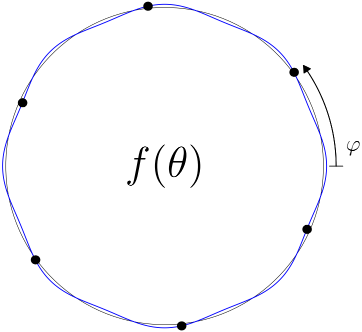

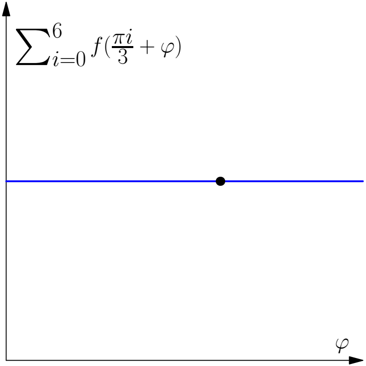

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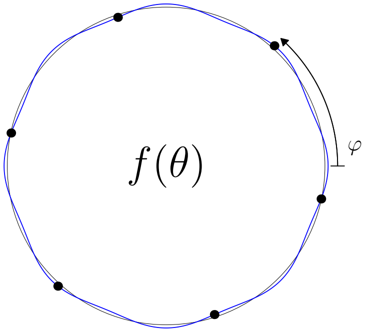

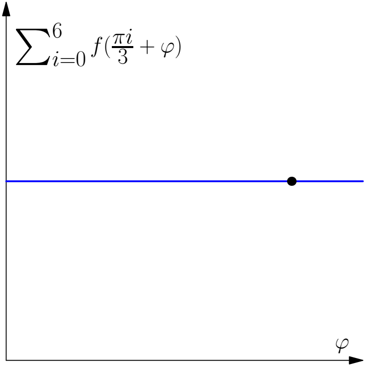

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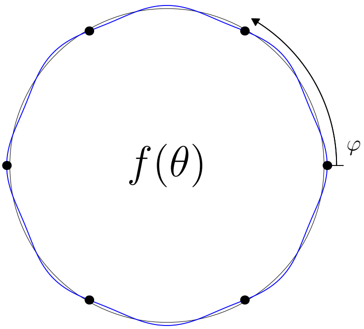

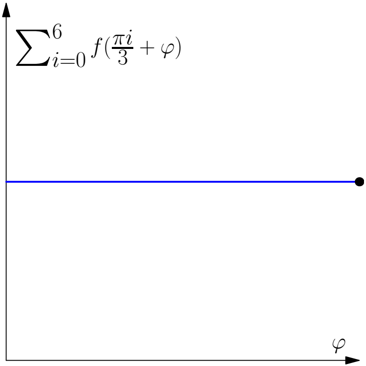

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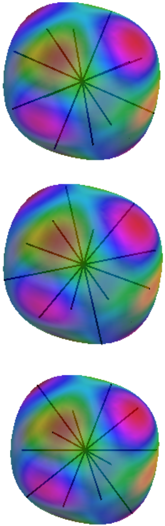
Why can we not improve over spheres?



Let $\mathbf{x}_i$, $i = 1, \ldots, 12$, be the twelve contact points on the sphere in the f.c.c. packing.

Lemma

Let f be an even function $S^2 \to \mathbb{R}$. $\sum_{i=1}^{12} f(R\mathbf{x}_i)$ is independent of $R \in SO(3)$ if and only if the expansion of $f(\mathbf{x})$ in spherical harmonics terminates at $l = 2$.

K, Adv Math 2014

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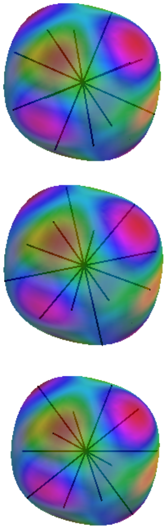

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Theorem (K)

The sphere is a local minimum of ϕ, the packing density, among convex, centrally symmetric bodies.

K, Adv Math 2014

Random close packing

Caveats:

- Protocol dependence, no single RCP density. We compare different shapes under same protocol
- Very elongated/flat particles pack much worse than spheres, so spheres can only ever be a local pessimum

$$p\Delta V = \sum_i \min_{R_i} \sum_{j\in\partial i} f_{ij}\Delta r(R_i\mathbf{n}_{ij}) + O(\Delta r^{3/2}),$$

$$\Delta r(\mathbf{u}) = \text{ deformation in direction } \mathbf{u}.$$

In RCP, every coordination shell is different, so even if for some, we manage to break even, for most we cannot.

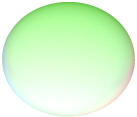
Result: $\phi - \phi_{\text{spheres}} > c\overline{|\Delta r(\mathbf{u}) - \overline{\Delta r(\mathbf{u})}|} + O(\overline{|\Delta r(\mathbf{u})|}^{3/2})$.

K, Soft Matter 2016

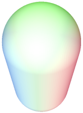
One-parameter shape families

Let $\rho = \overline{|\Delta r(\mathbf{u}) - \overline{\Delta r(\mathbf{u})}|}$, we can calculate $\eta = \frac{1}{3} d\phi / d\rho|_{\rho=0^+}$:

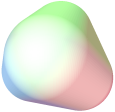
$\eta = 0.94$



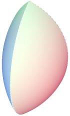
$\eta = 1.08$



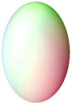
$\eta = 1.45$



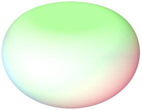
$\eta = 1.01$



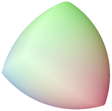
$\eta = 0.79$



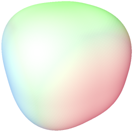
$\eta = 1.36$



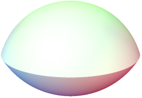
$\eta = 1.06$



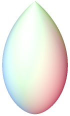
$\eta = 1.32$



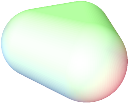
$\eta = 0.86$



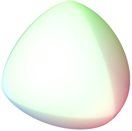
$\eta = 0.77$



$\eta = 1.31$



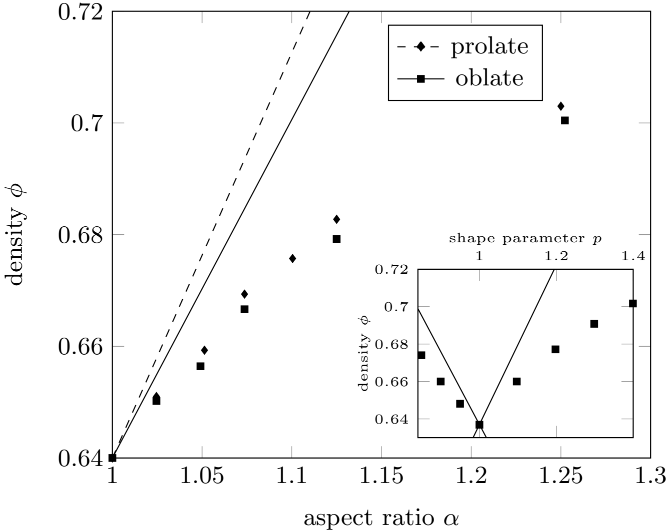
$\eta = 1.20$



End of slides

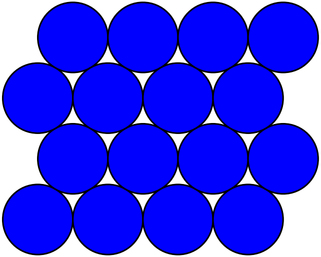
Back up slides follow

Comparison with simulation results



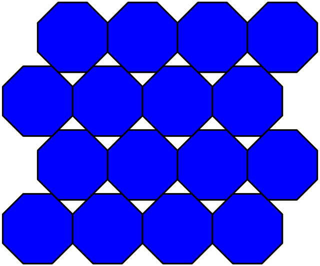
Main plot: ellipsoids; inset: superballs

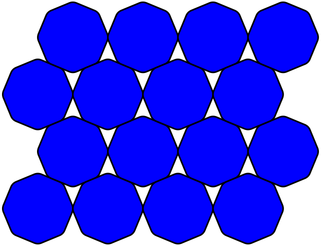
In 2D disks are not worst



$\phi =$ 0.9069

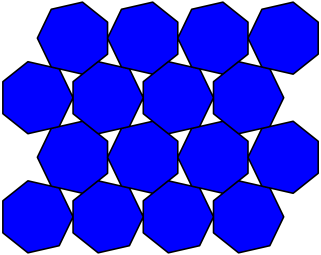
$\phi =$ 0.9062



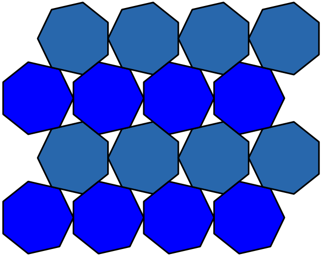


$\phi =$ 0.9024

$\phi =$ 0.8926(?)



Regular heptagon is locally worst packing (?)



0.8926(?)

Theorem (K)

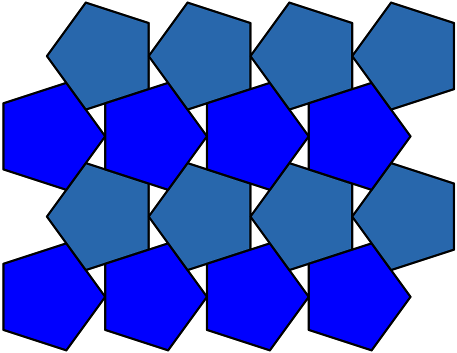
Any convex body sufficiently close to the regular heptagon can be packed at a filling fraction at least that of the "double lattice" packing of regular heptagons.

It is not proven, but highly likely, that the "double lattice" packing is the densest packing of regular heptagons.

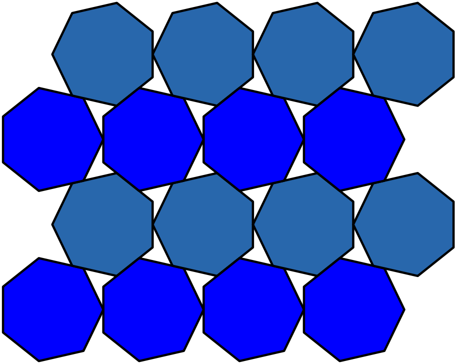
K, Geometry & Topology 2015

Local optimality of the double lattice packing

Work with Wöden Kusner (TU Graz)



$\phi = 0.9213$



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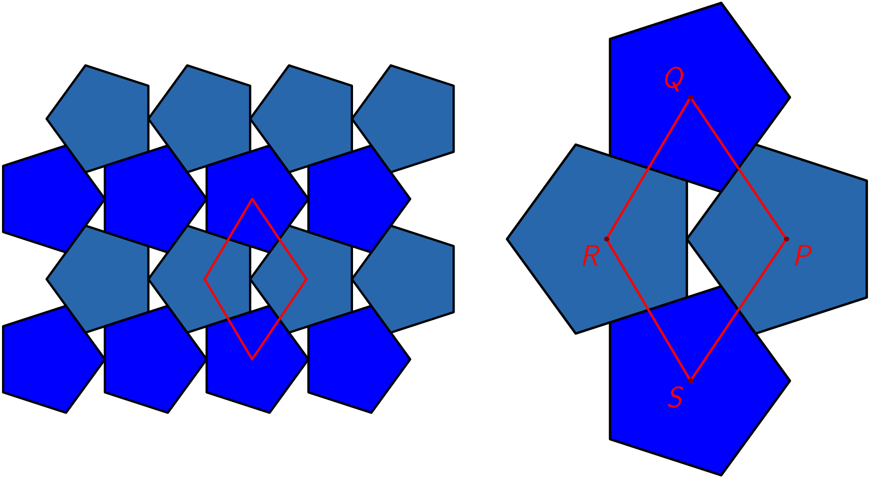
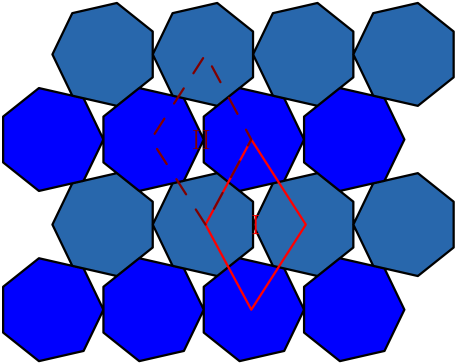
Pentagons

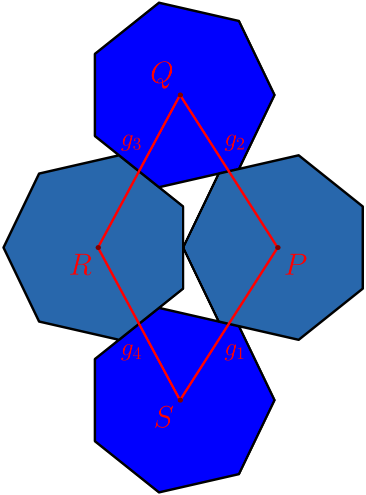


This configuration is a local minimum among nonoverlapping configurations of $\mathrm{area}(SPQR)$.

K and Kusner, arXiv:1509.02241

Heptagons

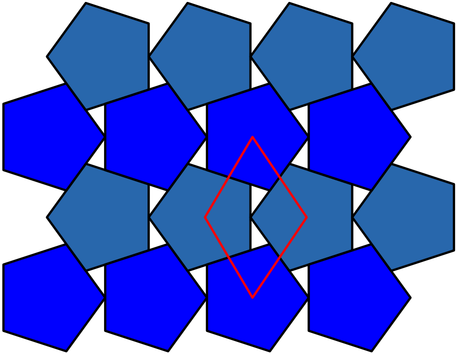




This configuration is not a local minimum of $\mathrm{area}(SPQR)$.
But it is a local minimum of $\mathrm{area}(SPQR) + \sum_{i=1}^{4} g_i$, where, e.g., $g_3^{(I)} + g_3^{(II)} = 0$.

K and Kusner, arXiv:1509.02241

Local optimality of the double lattice packing



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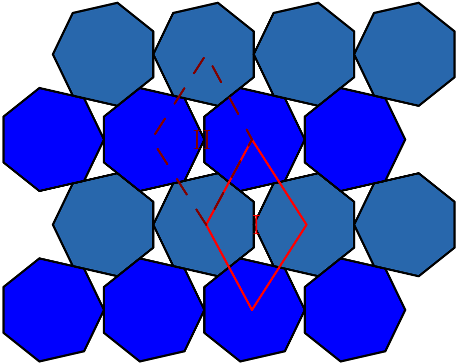

$\phi = 0.8926$

The same method that works for heptagons works for (almost) any convex polygon and shows the "double lattice" construction gives locally optimal packings.

K and Kusner, arXiv:1509.02241