Pessimal packing shapes

Yoav Kallus

Santa Fe Institute

AMS Special Session on Discrete Geometry and Convexity
For András Bezdek's 60th birthday)
Atlanta, January 6, 2017

Worst packing shapes

Best packing shapes are trivial

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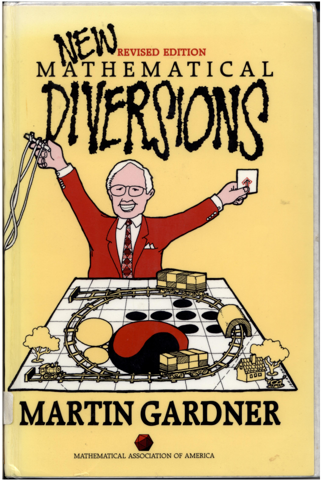
Worst shape is a more interesting question

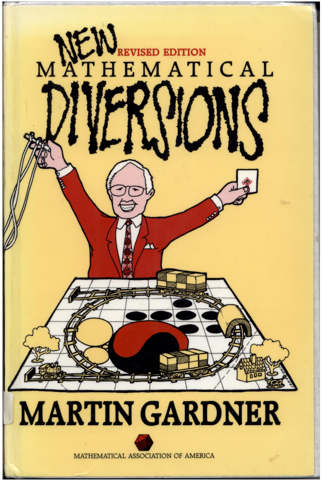
Ulam's Conjecture



"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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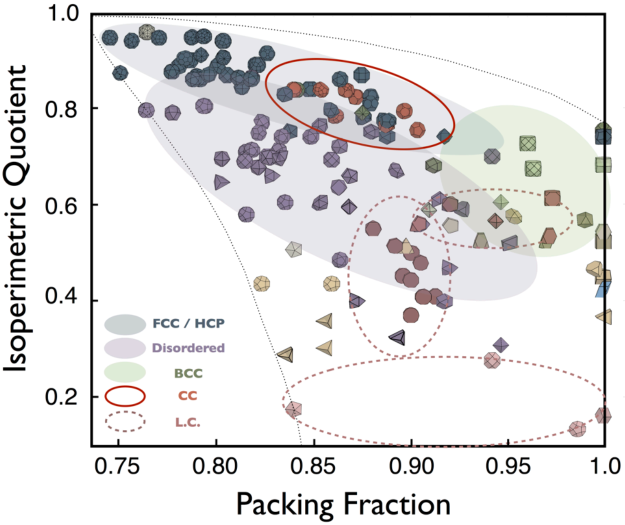
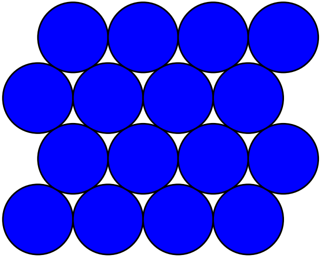
Packing convex shapes

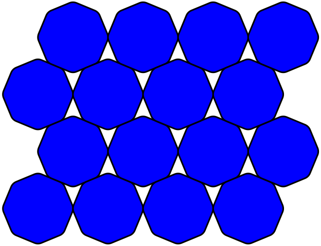


Damasceno, Engel, and Glotzer, 2012.

In 2D disks are not worst

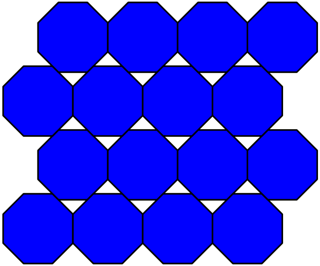


$\phi = 0.9069$

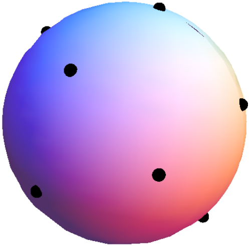


$\phi = 0.9024$

$\phi = 0.9062$



In what dimensions are spheres pessimal for lattice packing?

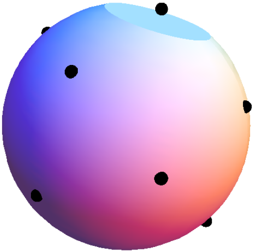


$\phi_L(B^n)$ is known for $n = 2, 3, 4, 5, 6, 7, 8$, and 24.

A lattice Λ that achieves a local maxmimum packing density is extreme. That is, there is ϵ s.t. when $||T - \mathrm{Id}|| < \epsilon$ then $\det T \geq 1$ or $||T\mathbf{x}|| < 1$ for some $\mathbf{x} \in \partial B^n \cap \Lambda$.

By linearization, Λ is extreme if and only if $\mathrm{Id} \in \mathrm{int\,cone}_{\mathbf{x}\in\partial B^n\cap\Lambda}\, \mathbf{x} \otimes \mathbf{x}$.

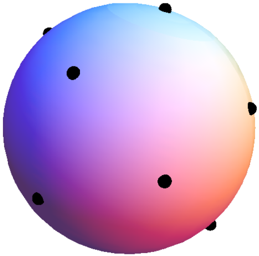
$n = 6, 7, 8, 24$

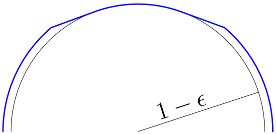


For $n = 6, 7, 8, 24$, the lattice Λ_n achieving $\phi_L(B^n)$ has a contact configuration W_n that is redundantly extreme: for any $W' = W_n \setminus \{\pm\mathbf{x}'\}$, we still have $\mathrm{Id} \in \operatorname{int}\operatorname{cone}_{\mathbf{x}\in W'} \mathbf{x} \otimes \mathbf{x}$.

Therefore, a slightly dented sphere B' has $\phi_L(B') < \phi_L(B^n)$.

$n = 4, 5$





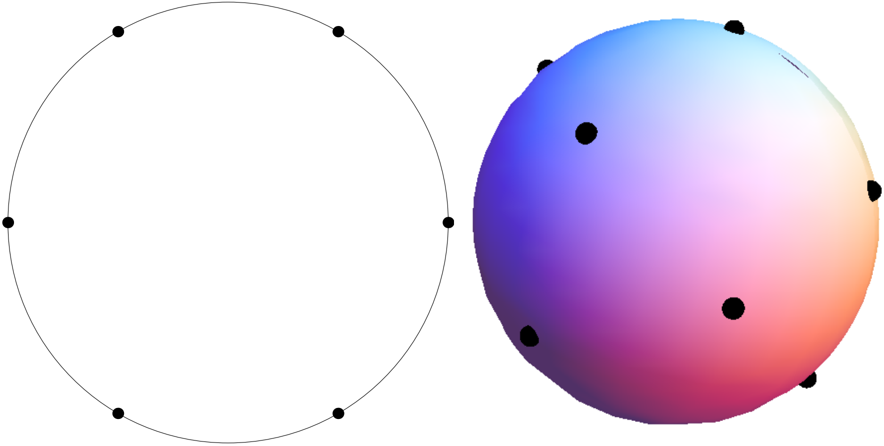
For $n = 4, 5$, the lattice Λ_n achieving $\phi_L(B^n)$ is nearly redundantly extreme: for any $W' = W_n \setminus \{\pm \mathbf{x}'\}$, we only have $\mathrm{Id} \in \partial \operatorname{cone}_{\mathbf{x} \in W'} \mathbf{x} \otimes \mathbf{x}$.

Therefore, there is ϵ such that when $\|T - \mathrm{Id}\| < \epsilon$, $T\mathbf{x} \geq 1$ for all but one $\mathbf{x} \in W_n$, then $\det T > 1 - C\|T - \mathrm{Id}\|^2$.

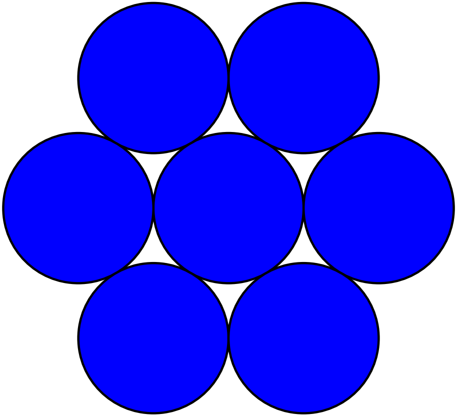
Consider the sphere "shaved" to a depth ϵ on two antipodal caps. Then $d_{B'} > (1 - C\epsilon^2) d_{B^n}$, $|B'| < (1 - c\epsilon)|B^n|$, and so so $\phi_L(B') < \phi_L(B^n)$.

$n = 2, 3$

For $n = 2, 3$, we have that $\{\mathbf{x} \otimes \mathbf{x} : \mathbf{x} \in W_n\}$ is a basis for Sym^n. So any deformation of the boundary is matched by a proportional changed in the critical determinant.



Why can we improve over circles?



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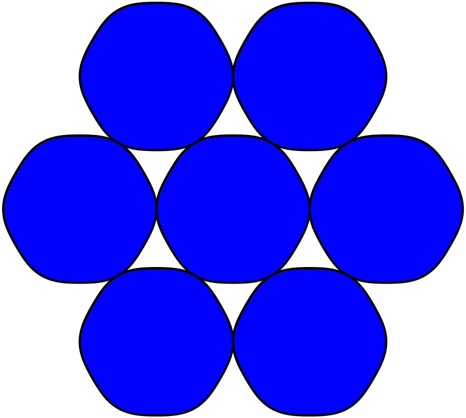

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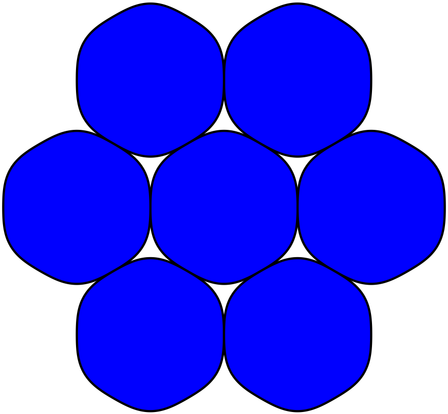

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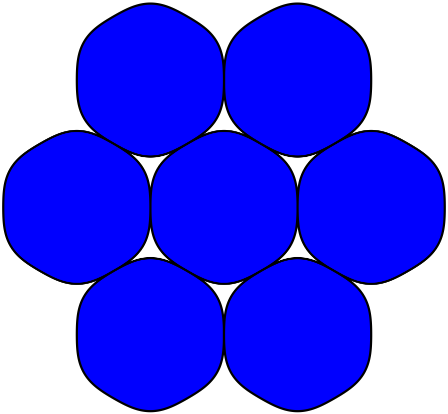

To first order:

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.

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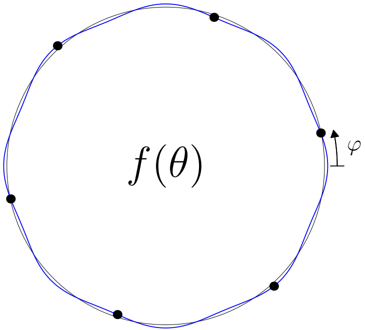

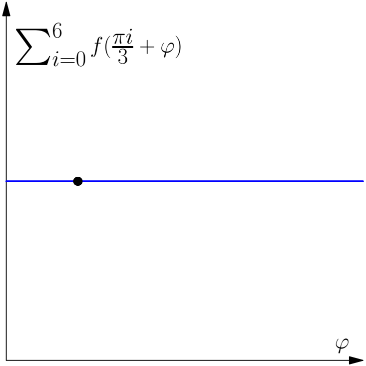

$f(\theta) = 1 + \epsilon cos(8\theta)$

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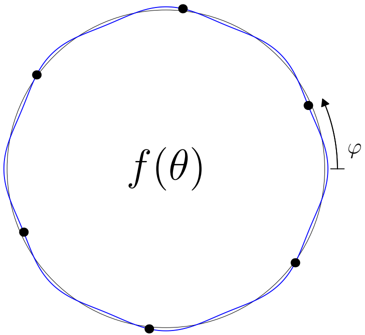

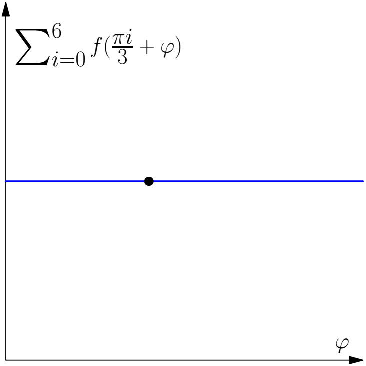

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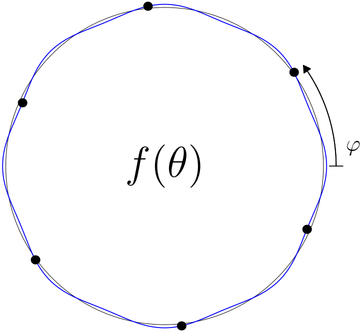

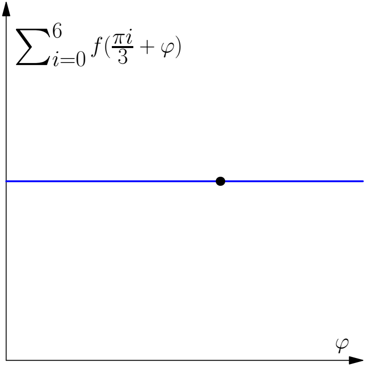

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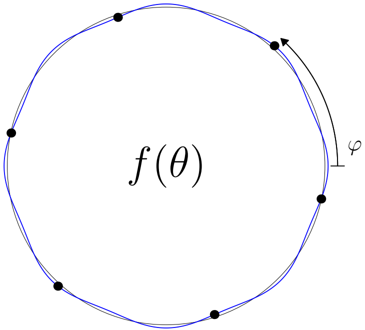

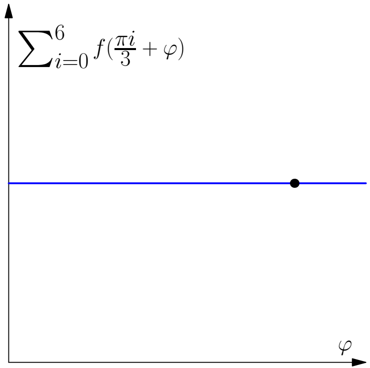

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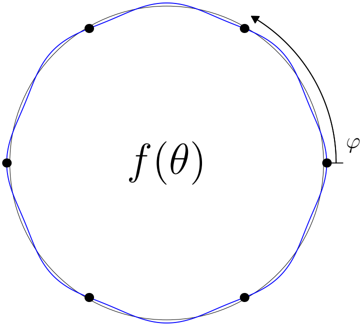
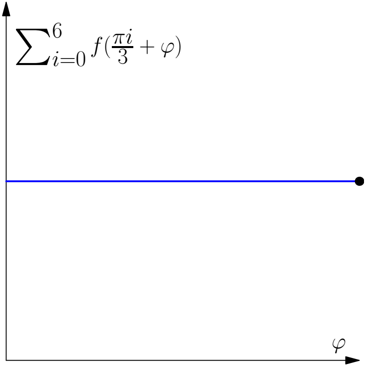
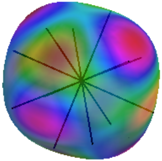
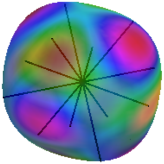


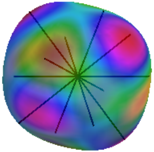


$f(\theta) = 1 + \epsilon cos(8\theta)$

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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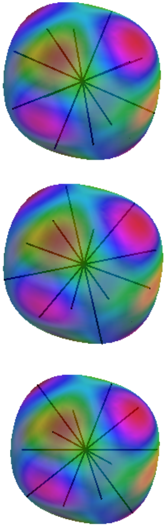

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Theorem (K)

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, <u>for most we cannot.</u>

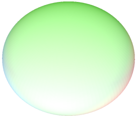
Result: $\phi - \phi_{\text{spheres}} > c\overline{|\Delta r(\mathbf{u}) - \overline{\Delta r(\mathbf{u})}|} + O(\overline{|\Delta r(\mathbf{u})|}^{3/2})$.

K, Soft Matter 2016

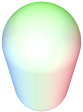
One-parameter shape families

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

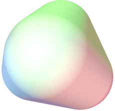
$\eta = 0.94$



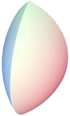
$\eta = 1.08$



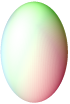
$\eta = 1.45$



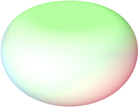
$\eta = 1.01$



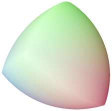
$\eta = 0.79$



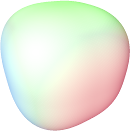
$\eta = 1.36$



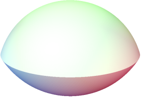
$\eta = 1.06$



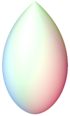
$\eta = 1.32$



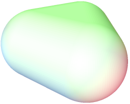
$\eta = 0.86$



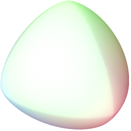
$\eta = 0.77$



$\eta = 1.31$



$\eta = 1.20$



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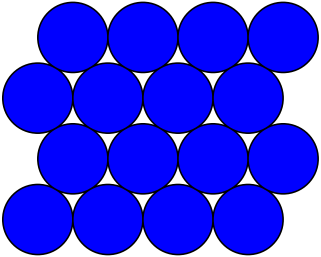

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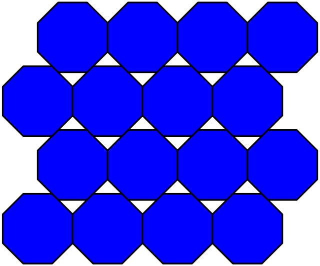

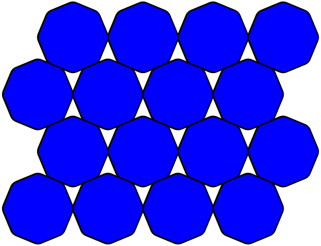

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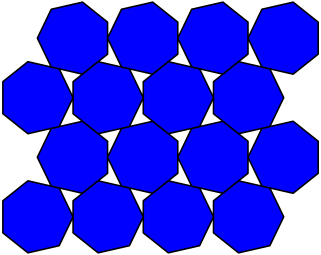
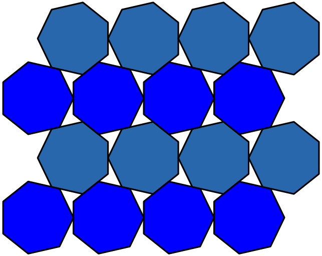


Regular heptagon is locally worst packing (?)



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