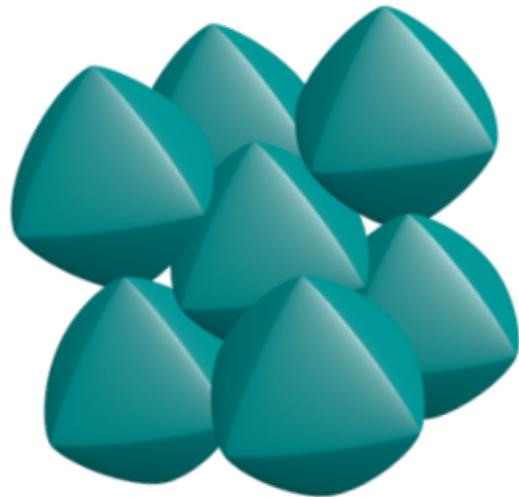


Packings of Superballs



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Computational Challenges in the Theory of Lattices
April 25, 2018



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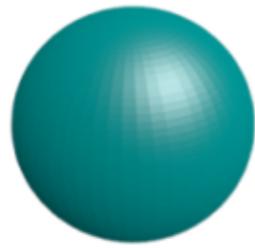


Packings of superballs

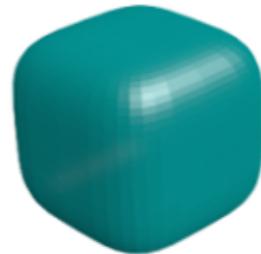
$$B_3^p = \{(x, y, z) \in \mathbb{R}^3 : |x|^p + |y|^p + |z|^p \leq 1\}$$



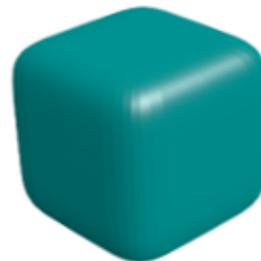
$p=1$



$p=2$



$p=4$



$p=6$



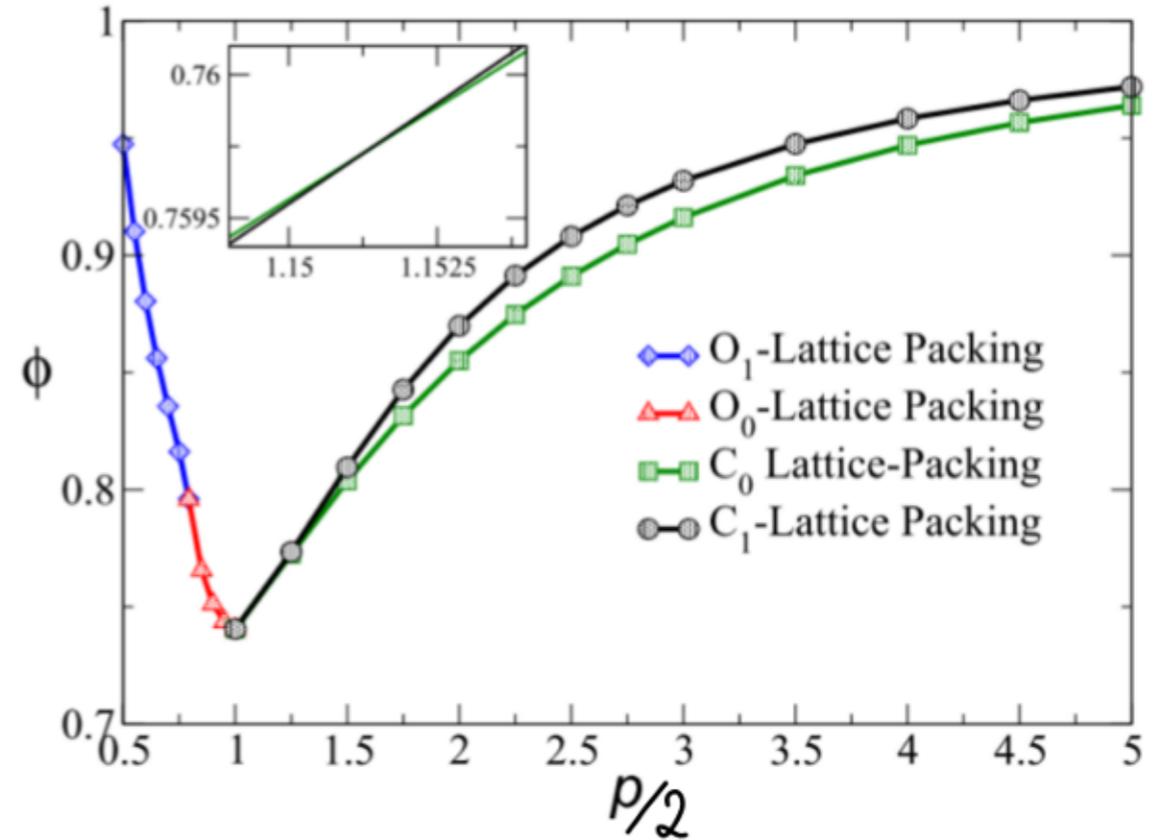
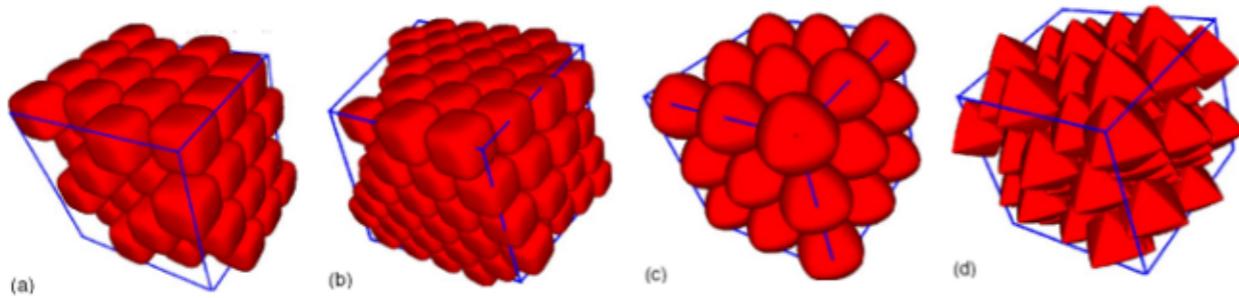
$p=8$

Conjecture (Torquato, Jiao, 2009): "Kepler's conjecture for the 21st century"

Densest packings of centrally symmetric Platonic, Archimedean solids, and of L^p -unit balls are given by the corresponding lattice packing.

Numerical Simulation

Jiao, Stillinger, Torquato (2009)
identify four families of packings



"The existence of the continuous "path" of superball packings that we found connecting the FCC lattice packing of spheres and the Minkowski-lattice packing of regular octahedra provides strong evidence that our candidate packings are very likely optimal."

Numerical Simulation

Ni, Gantapara, de Graaf, van Rooij, Dijkstra (2012)



found improved superball packings for $p \in [\log_2 3, 2]$ and $p = 1.4$

Lattice packings

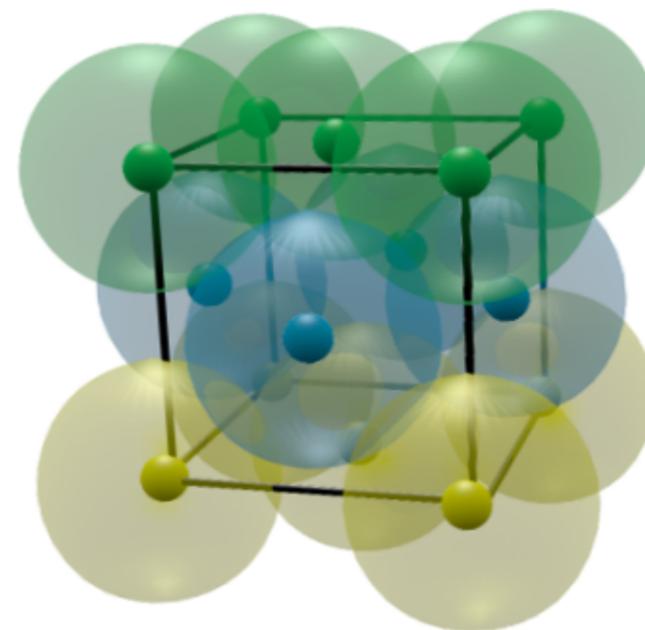
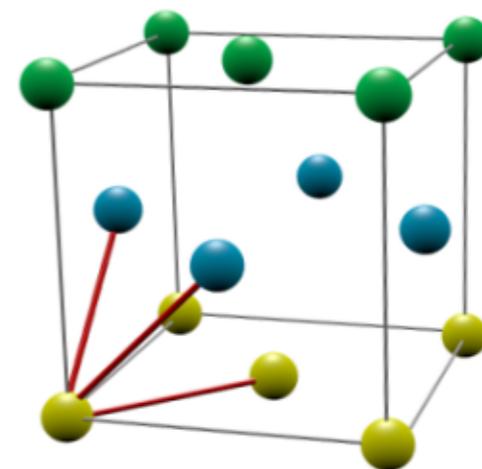
Let $\Delta(K) = b_1\mathbb{Z} \oplus b_2\mathbb{Z} \oplus b_3\mathbb{Z}$ with $b_1, b_2, b_3 \in \mathbb{R}^3$
be a packing lattice for K .

$v-w \notin K^\circ - K^\circ$ for all $v, w \in \Delta(K)$ with $v \neq w$.

Lattice packing density

$$\delta^2(K) = \max \left\{ \frac{\text{vol } K}{\det \Delta(K)} : \Delta(K) \text{ packing lattice of } K \right\}$$

$\det \Delta(K) = \text{volume of fundamental domain}$



Optimal lattice packings

Minkowski (1904):

Method to find densest lattice packings for convex bodies $K \subseteq \mathbb{R}^3$

determined densest packings for octahedron B_3^1



$$\delta^e(B_3^p) = \max \left\{ \frac{\text{vol } B_3^p}{|\det B|} : B \in GL_3(\mathbb{R}) \text{ basis of packing lattice for } B_3^p \right\}$$

equivalently

minimize $|\det B|$

such that $B \in GL_3(\mathbb{R}) \setminus GL_3(\mathbb{Z})$

$\|Bv\|_p \geq 2$ for all $v \in \mathbb{Z}^3 \setminus \{0\}$

Minkowski's method

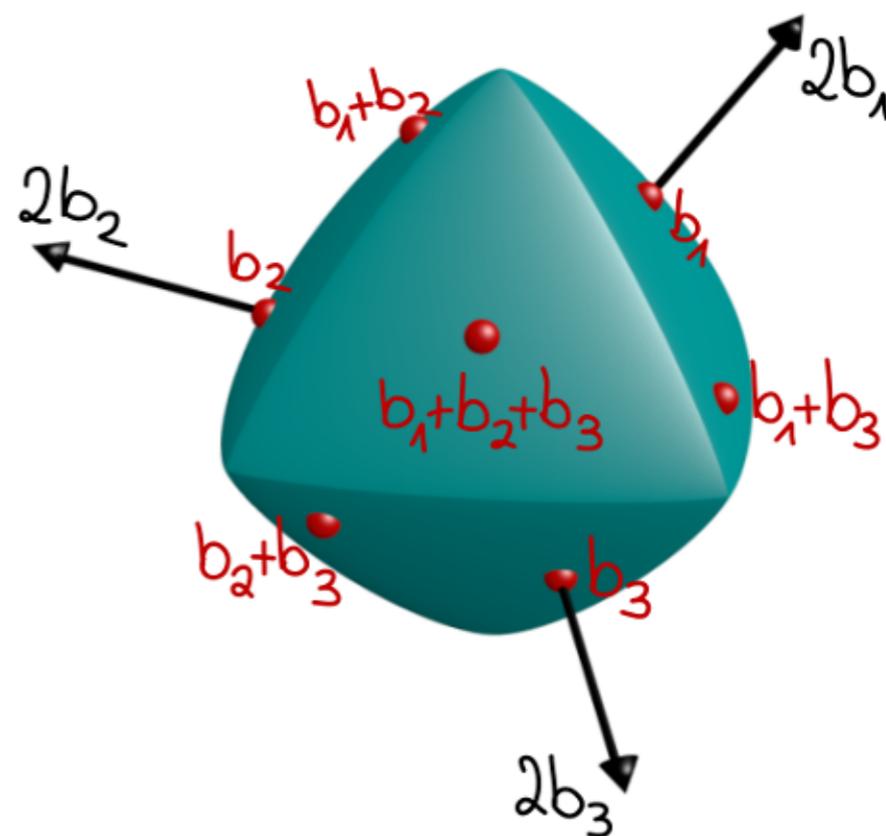
If B gives locally densest lattice packing, then number of $v \in \mathbb{Z}^3$ with $\|Bv\|_p = 2$ is either 12 or 14.

After performing a $GL_3(\mathbb{Z})$ -transformation we can assume that exactly the following $v \in \mathbb{Z}^3$ satisfy $\|Bv\|_p = 2$

$$\text{Case I: } \pm \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ -1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}$$

$$\text{Case II: } \pm \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\text{Case III: } \pm \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$



Betke & Henk (2000): Developed algorithm for K -polytope

Locally optimal solutions

Let x^* be a feasible solution of the following problem

$$\min (\det X)^2$$

$$X \in \mathbb{R}^{3 \times 3}$$

$$\|Xv\|_p = 2 \quad \text{for all } v \in \mathcal{U}$$

and $\mu^* \in \mathbb{R}^{|\mathcal{U}|}$ such that

$$\nabla_X \mathcal{L}(X^*, \mu^*) = 0 \quad \text{with } \mathcal{L}(X, \mu) = (\det X)^2 + \sum_{v \in \mathcal{U}} \mu_v (\|Xv\|_p - 2)$$

and

$$y^T (\nabla_X^2 \mathcal{L}(X^*, \mu^*)) y > 0 \quad \text{for all } y \in \mathbb{R}^9 \text{ with } y \neq 0 \text{ and}$$
$$y^T \nabla_{X^*} (\|X^*v\|_p - 2) = 0 \quad \forall v \in \mathcal{U}$$

then X^* is a locally optimal solution.

Shortest vector

Lemma (Dieter 1975)

Let $b_1, \dots, b_n \in \mathbb{R}^n$ be a basis of a lattice Δ and let $\mu, p \in \mathbb{R}$. A lattice point $v = \sum_{i=1}^n \alpha_i b_i$ with $\alpha_i \in \mathbb{Z}$ and $\|v\|_p \leq \mu$ has to satisfy

$$|\alpha_i| \leq \mu \sqrt[n]{G_{ii}^{-1}} \quad \forall i \in \{1, \dots, n\}$$

where G is the Gram matrix of Δ given by $G_{ij} = \langle b_i, b_j \rangle$.

Results

use nonlinear optimization:

- Newton's method
- Check KKT conditions
- Check shortest vectors

Four regimes:

$p \in [1, \log_2 3]$: Case III new family including Minkowski's lattice

$$B = \begin{pmatrix} -x & z & y \\ y & -x & z \\ z & y & -x \end{pmatrix} \quad x, y, z > 0 \quad \|B\|_p = 1$$

$p \in [\log_2 3, 2]$: Case I bct lattices of Ni, Gantapara, de Graaf, ...

$p \in [2, 2.3018\dots]$: Case I C_0 lattice of Jiao, Stillinger, Torquato

$p \in [2.3018\dots, \infty)$: Case I C_1 lattice of Jiao, Stillinger, Torquato

Existence of lattices

Theorem (Cohn, Kumar, Minton 2015)

Let V and W be finite-dimensional normed vector spaces over \mathbb{R} , and suppose that $f: B(x_0, \varepsilon) \rightarrow W$ is a C^1 -function, where $x_0 \in V$, $\varepsilon > 0$.

Suppose also that $T: W \rightarrow V$ is a linear operator such that

$$\|Df(x) \circ T - \text{id}_W\| < 1 - \frac{\|T\| \cdot |f(x_0)|}{\varepsilon}$$

for all $x \in B(x_0, \varepsilon)$. Then there exists $x_* \in B(x_0, \varepsilon)$ such that $f(x_*) = 0$.

Moreover, in $B(x_0, \varepsilon)$, the zero locus $f^{-1}(0)$ is a C^1 submanifold of dimension $\dim V - \dim W$.

$$f(p, x, y, z) = \begin{pmatrix} 3(-x+y+z)^p - 1 \\ x^p + y^p + z^p - 1 \\ (x-y)^p + (z+y)^p + (z-x)^p - 1 \end{pmatrix}$$

$$T = Df'(p_0, x_0, y_0, z_0)^+$$

Family of packing lattices

For $p \in [1, \log_2 3]$ the lattice $\Delta = 2b_1\mathbb{Z} \oplus 2b_2\mathbb{Z} \oplus 2b_3\mathbb{Z}$ with $b_1 = \begin{pmatrix} -x \\ y \\ z \end{pmatrix}$, $b_2 = \begin{pmatrix} z \\ -x \\ y \end{pmatrix}$, $b_3 = \begin{pmatrix} y \\ z \\ -x \end{pmatrix}$ where $z \geq x \geq y > 0$ such that $3(-x+y+z)^p = 1$, $x^p + y^p + z^p = 1$, and $(x-y)^p + (z+y)^p + (z-x)^p = 1$ is a packing lattice.

Proof: Hanner's inequality: $\|f+g\|_p^p + \|f-g\|_p^p \geq |\|f\|_p + \|g\|_p|^p + |\|f\|_p - \|g\|_p|^p$ for $p \in [1, 2]$

We know: Δ satisfies Case III: $\|Bv\|_p^p = 1$ for $v \in \{\pm \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\}$

Let $v = \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$: $\|B \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}\|_p^p \geq |\|B \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\|_p + \|B \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}\|_p|^p + |\|B \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\|_p - \|B \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}\|_p|^p - \|B \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}\|_p^p \geq 2^p - 1 \geq 1$

Analogously for all remaining $v \in \{0, \pm 1\}^3$

If $\|Bv\|_p \geq 1$ for $v \in \{0, \dots, \pm d\}^3$ then $\|Bv\|_p \geq 1$ for $v \in \{0, \dots, \pm (d+1)\}^3$

Upper bounds

Theorem (Cohn, Elkies 2003)

$$\delta^+(K) \leq \inf f(0)$$

$$f \in S(\mathbb{R}^n)$$

$$\hat{f}(0) \geq \text{vol } K$$

$$\hat{f}(u) \geq 0 \text{ for all } u \in \mathbb{R}^n \setminus \{0\}$$

$$f(x) \leq 0 \text{ for all } x \in K^\circ - K^\circ$$



Fourier transform of f :
$$\hat{f}(u) = \int_{\mathbb{R}^n} f(x) e^{-2\pi i x \cdot u} dx$$

Upper bounds

Theorem (Cohn, Elkies 2003)

$$\delta^t(K) \leq \inf f(0)$$

$$f \in S(\mathbb{R}^n)$$

$$\hat{f}(0) \geq \text{vol } K$$

$$\hat{f}(u) \geq 0 \text{ for all } u \in \mathbb{R}^n \setminus \{0\}$$

$$f(x) \leq 0 \text{ for all } x \in K^\circ - K^\circ$$

SET $\hat{f}(u) = p(u) e^{-\pi \|u\|^2}$

$$\delta^t(K) \leq \inf \int_{\mathbb{R}^n} p(u) e^{-\pi \|u\|^2} du$$

$$p \in \mathbb{R}[u]_{\leq 2d}$$

$$p(0) \geq \text{vol } K$$

$$p(u) \geq 0 \text{ for all } u \in \mathbb{R}^n \setminus \{0\}$$

$$\int_{\mathbb{R}^n} p(u) e^{-\pi \|u\|^2} e^{2\pi i u \cdot x} du \leq 0 \text{ for all } x \in K^\circ - K^\circ$$

Fourier transform of f : $\hat{f}(u) = \int_{\mathbb{R}^n} f(x) e^{-2\pi i x \cdot u} dx$

Solving the optimization problem

$$\delta^t(K) \leq \inf_{\mathbb{R}^n} \int p(u) e^{-\pi \|u\|^2} du$$

$$p \in \mathbb{R}[u]_{\leq 2d}$$

$$p(0) \geq \text{vol } K$$

$$p(u) \geq 0 \text{ for all } u \in \mathbb{R}^n \setminus \{0\}$$

← NP-hard condition

$$\int_{\mathbb{R}^n} p(u) e^{-\pi \|u\|^2} e^{2\pi i u \cdot x} du \leq 0 \text{ for all } x \notin K^\circ - K^\circ$$

SEMIDEFINITE RELAXATION: SUM OF SQUARES (SOS)

$$- p \in \mathbb{R}[u]_{2d} \text{ is SOS: } p = q_1^2 + \dots + q_m^2 \Leftrightarrow \exists Q \in \mathcal{S}_{\geq 0}^{\binom{n+d}{d}} : p(u) = [u]_d^T Q [u]_d = \langle [u]_d [u]_d^T, Q \rangle$$

Solving the optimization problem

$$\delta^t(K) \leq \inf_{\mathbb{R}^n} \int p(u) e^{-\pi \|u\|^2} du$$

$$p \in \mathbb{R}[u]_{\leq 2d}$$

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SEMIDEFINITE RELAXATION: SUM OF SQUARES (SOS)

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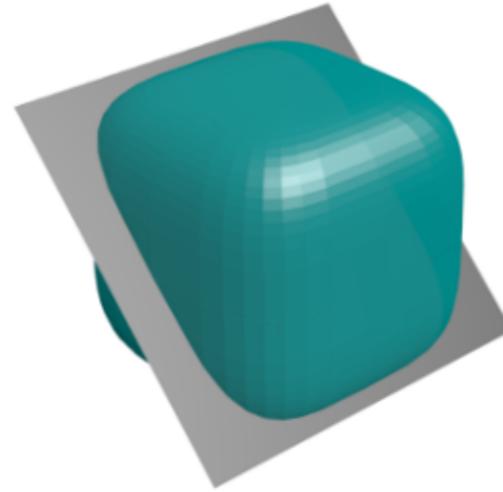
- if $n=3, d=15$, then $Q \in \mathcal{S}_{\geq 0}^{816}$; too big for current SDP solvers

IDEA: WE CAN ASSUME THAT p IS INVARIANT UNDER SYMMETRY GROUP OF $K-K$

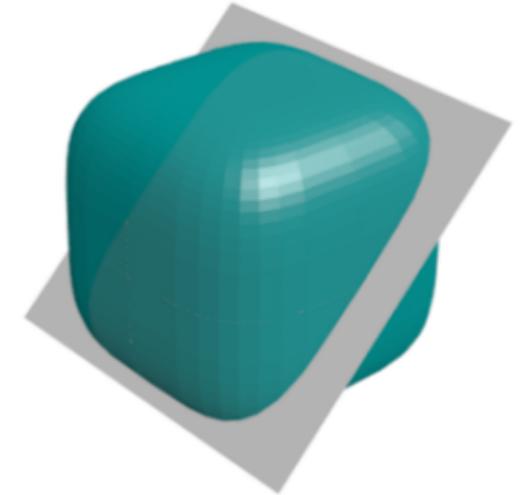
Finite reflection group



$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$$

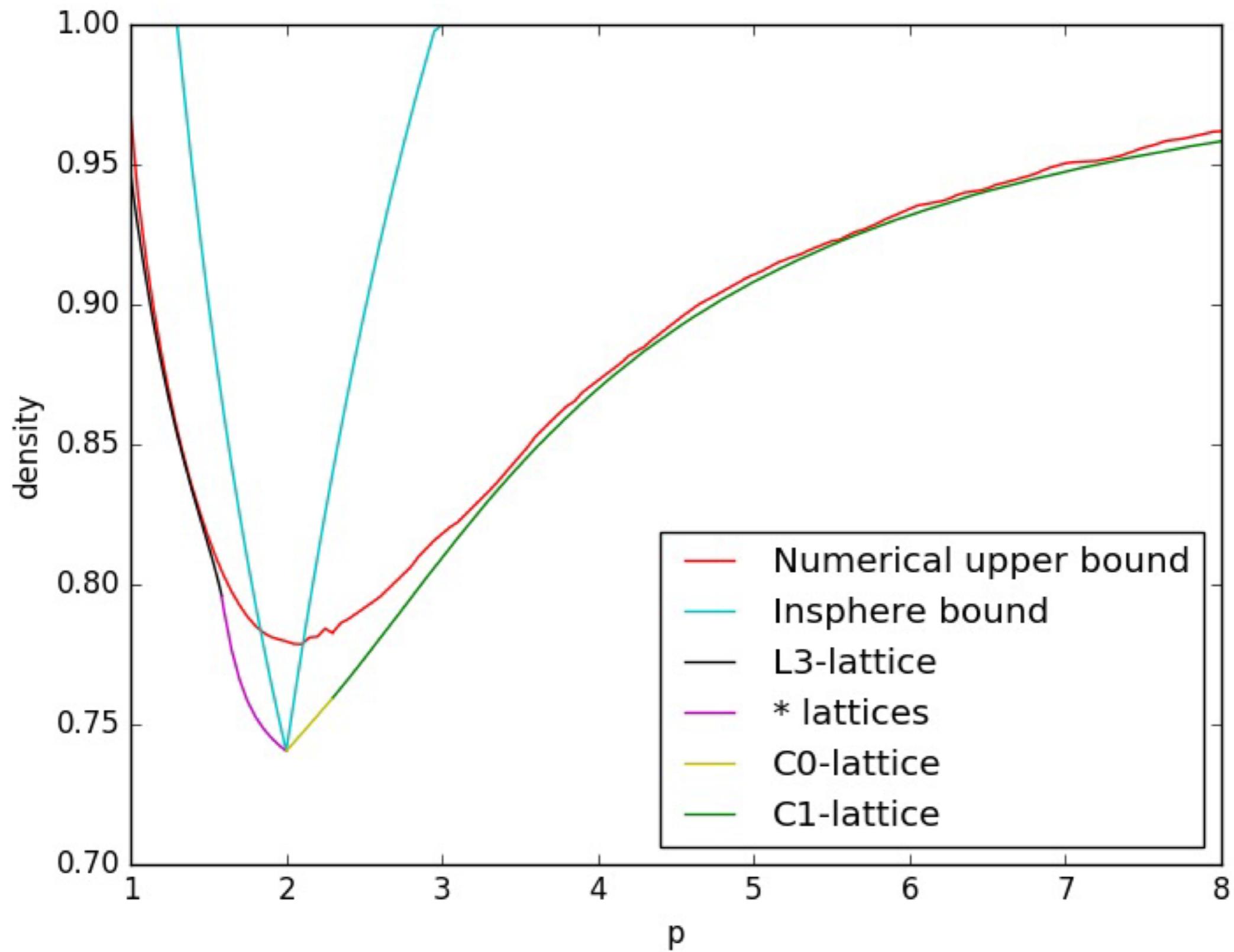


$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Reflection group B_3 , 48 elements

can assume

$$\bar{\rho}(\pm X_{\sigma(1)}, \pm X_{\sigma(2)}, \pm X_{\sigma(3)}) = \bar{\rho}(X_{\lambda_1}, X_{\lambda_2}, X_{\lambda_3})$$



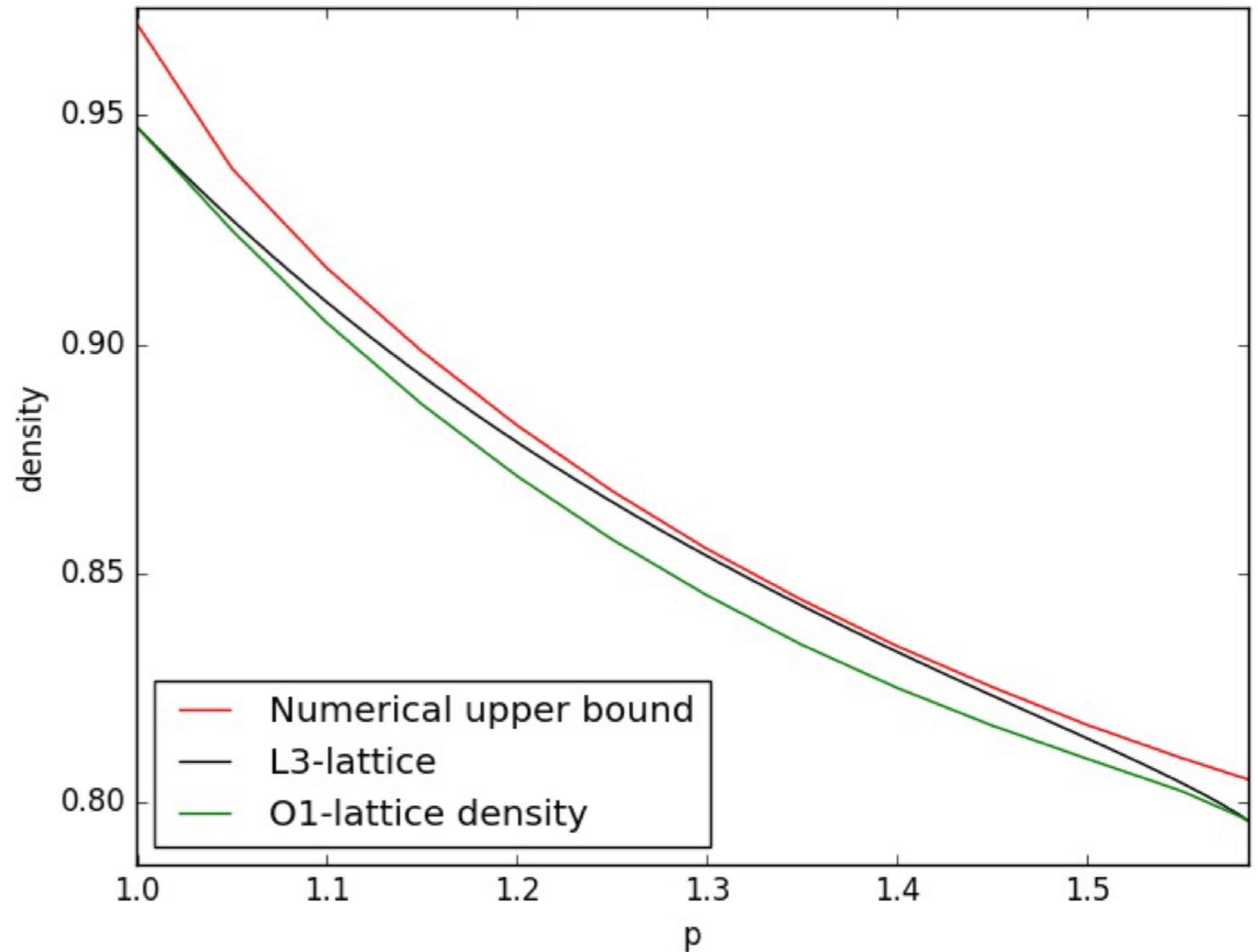
First regime

Best result for $p \in [1, \log_2 3]$:

$$L_3: \begin{aligned} b_1 &= 2(-x, y, z), \\ b_2 &= 2(z, -x, y), \\ b_3 &= 2(y, z, -x) \end{aligned}$$

$$\begin{aligned} x, y, z \in \mathbb{R}_{>0}: \quad & z = 3^{-\frac{1}{p}} + x - y \\ & x^p + y^p + z^p = 1 \\ & (y-x)^p + (3^{-\frac{1}{p}} + x)^p + (3^{-\frac{1}{p}} - y)^p = 1 \\ & z \geq x \geq y \end{aligned}$$

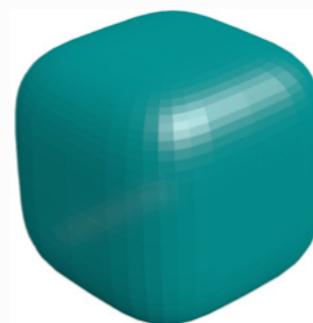
Case III \Rightarrow 14 contact points



Computational results

$p=2$: coincides with upper bound of Cohn & Elkies

$p=1,3,4,5,6$: new upper bounds



p :

1

2

3

4

5

6

LOWER
BOUNDS:

0,9473

0,7404

0,8095

0,8698

0,9080

0,9318

UPPER
BOUNDS:

0,9729

0,7797

0,8236

0,8742

0,9224

0,9338

THANK YOU FOR YOUR

ATTENTION!