# Numerical search methods for dense sphere packings in higher dimensions

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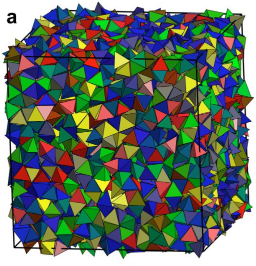
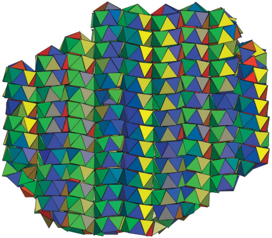
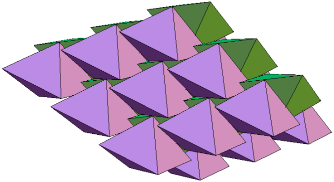
# From Hilbert's 18$^{th}$ Problem

"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?" (emphasis added)

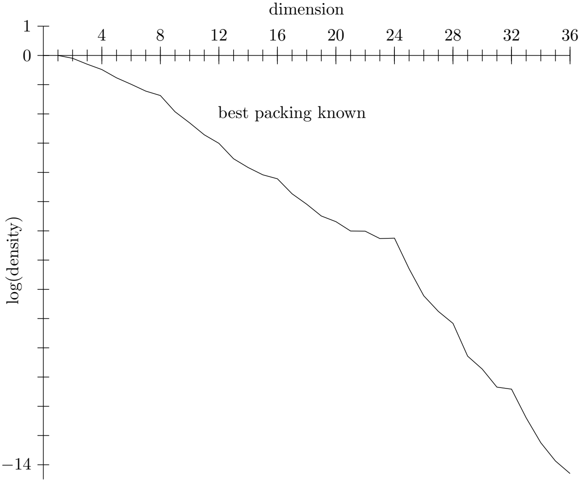
# Packing tetrahedra can get weird





# Densest known packing for $d \leq 36$




Recently solved in $d = 8, 24$, still open for all other $d > 3$.

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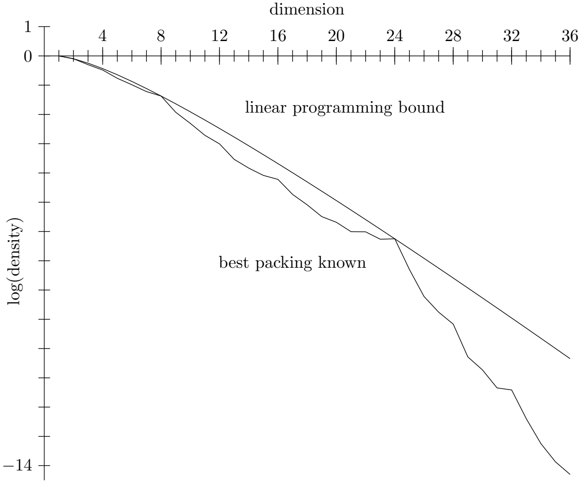
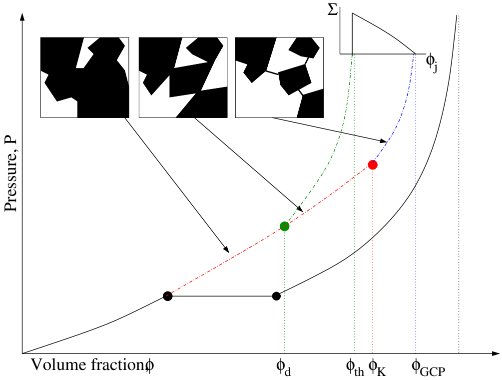


# Replica symmetry breaking solution of the hard sphere glass transition for $d \to \infty$

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$\phi_{GCP} \sim d \log(d) 2^{-d}$,
$\phi_{\text{opt}} \sim ?$

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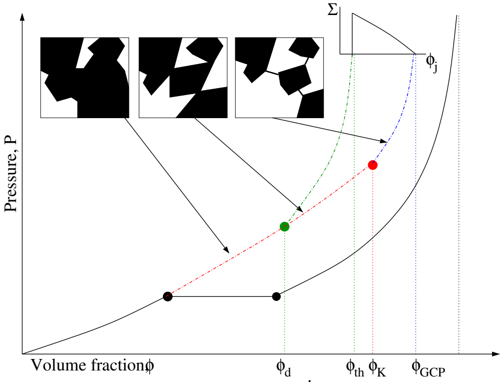


$\phi_{th} \sim d2^{-d}$,
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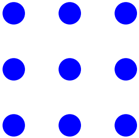
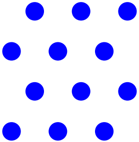
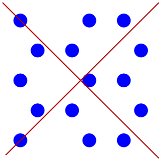
$\phi_{\mathrm{opt}} \sim ?$

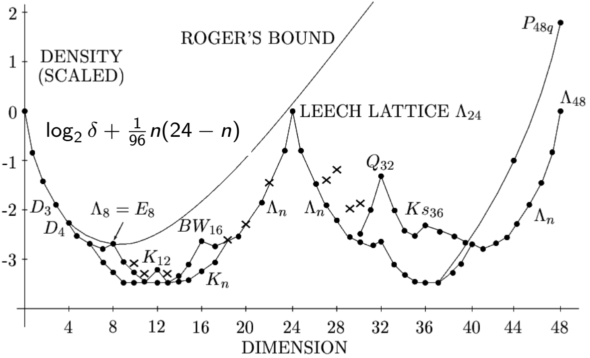
Minkowski: $\phi_{\mathrm{opt}} \gtrsim 2^{-d}$; others: $\phi_{\mathrm{opt}} \gtrsim d2^{-d}$ for all $d$, and $\phi_{\mathrm{opt}} \gtrsim d \log(\log d) 2^{-d}$ for some subseq. $d \to \infty$.
Kabatiansky–Levenshtein: $\phi_{\mathrm{opt}} \lesssim 2^{-0.5990d}$

# Bravais lattices



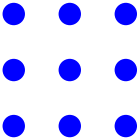




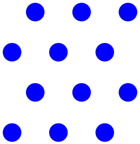



Bravais lattice is densest known packing in 26 out of first 36 dimensions.

# Packings with fixed number of translational orbits



$m = 1$



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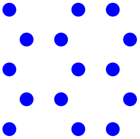
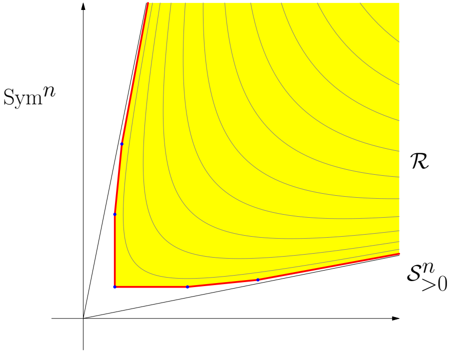


$m = 2$

$\lim_{m\to\infty} \phi_{d,m} = \phi_d$

# Enumeration of locally optimal lattices

Lattice: $\Lambda = \{A\mathbf{n} : \mathbf{n} \in \mathbb{Z}^d\}$, $A \sim d \times d$.
Let $G = A^T A$, then $\Lambda$ has packing radius $\geq 1$ if $\mathbf{n}^T G \mathbf{n} \geq 2$ for all $\mathbf{n} \in \mathbb{Z}^d$.
det $G$ is quasiconcave.




Also, invariant under $G \mapsto UGU^T$ when $U \in GL_n(\mathbb{Z})$.

# Results of enumeration

| dimension | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|
| # verts. | 1 | 1 | 2 | 3 | 7 | 33 | 10916 | $> 10^9$ |
| # locally opt. | 1 | 1 | 2 | 3 | 6 | 30 | 2408 | |

# What breaks for $m = 2$?

Double lattice: $\Lambda = \left\{A\mathbf{n} : \mathbf{n} \in \mathbb{Z}^d \times \{0,1\}\right\}$, $A \sim d \times (d+1)$.
Let $G = A^T A$, then $\Lambda$ has packing radius $\geq 1$ if $\mathbf{n}^T G \mathbf{n} \geq 2$ for all $\mathbf{n} \in \mathbb{Z}^d \times \{-1, 0, 1\}$.
$\det G_{1\ldots d, 1\ldots d}$ is quasiconcave.
But constraint $\operatorname{rank} G = d$ is nonlinear.

Weird things can happen: $D_9 \cup (D_9 + (\frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2}, t))$ is locally optimal for all $t$ (because $D_9$ by itself is already locally optimal).

# Enumeration of double-lattices ($m = 2$)

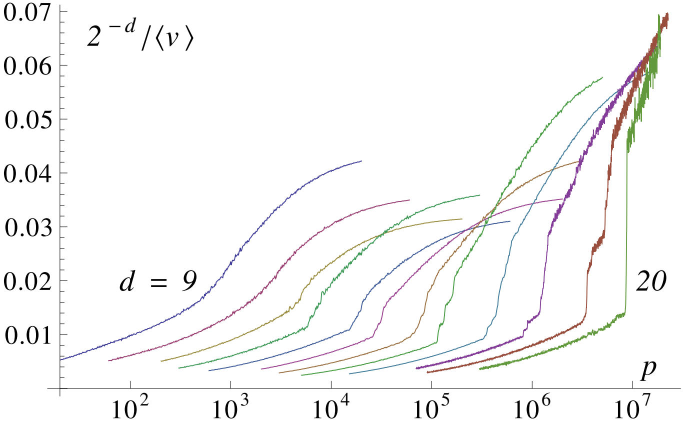
Let $\mathcal{R} = \{G \in \mathrm{S}ym^d : \mathbf{n}^T G \mathbf{n} \geq 2$ for all $\mathbf{n} \in \mathbb{Z}^d \times \{-1, 0, 1\}$.
Let $\mathcal{R}_0 = \{G \in \mathcal{R} : \mathrm{rank}\, G = d\}$.
Then local optima of det $G_{1\ldots d, 1\ldots d}$ within $\mathcal{R}_0$ either (1) lie on edges of $\mathcal{R}$, or (2) are two translates of a lattice that is already locally optimal.

# Results of enumeration ($m = 2$)

| dimension | 3 | 4 | 5 |
|---|---|---|---|
| # vertices of $\mathcal{R}$ | 4 | 10 | 34 |
| # pts. in $\mathcal{R}_0$ on edges of $\mathcal{R}$ | 3 (1) | 7 (3) | 31+full edge (23) |
| # locally optimal | 3 (1) | 7 (3) | 29 (20) |
| degen. of global opt. | 3 (1) | 2 (0) | 5 (2) |
| total (non-lattice) | | | |

*Andreanov & K, in prep.*

# Thermodynamically sampling lattices




Prob. $\sim \exp(-pV_{\text{unit cell}})$

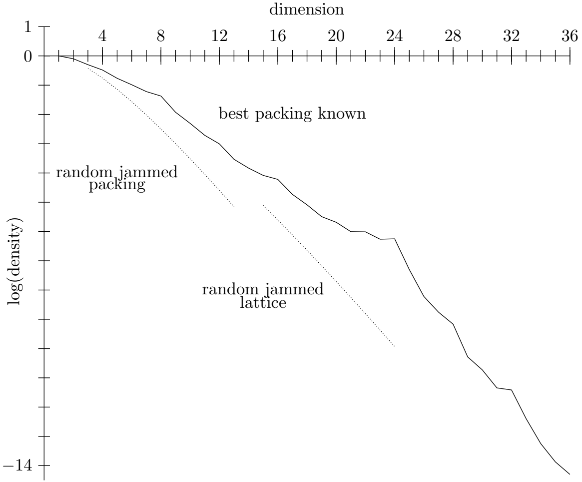
Densest known lattice recovered in some runs for $d \leq 20$

Can easily be extended to $m > 1$.

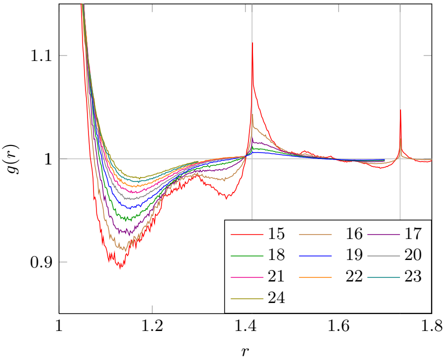
*K, Phys. Rev. E 87, 063307 (2013)*

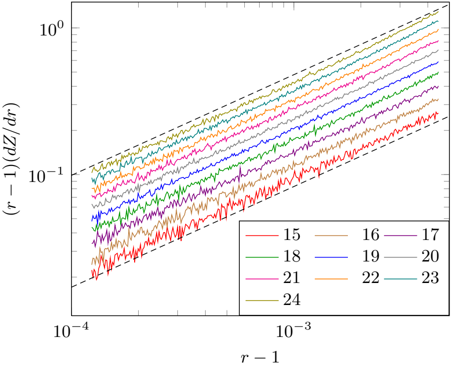
# Lattice RCP

$\phi \sim d^2 2^{-d}$?



# Pair correlations and quasicontacts

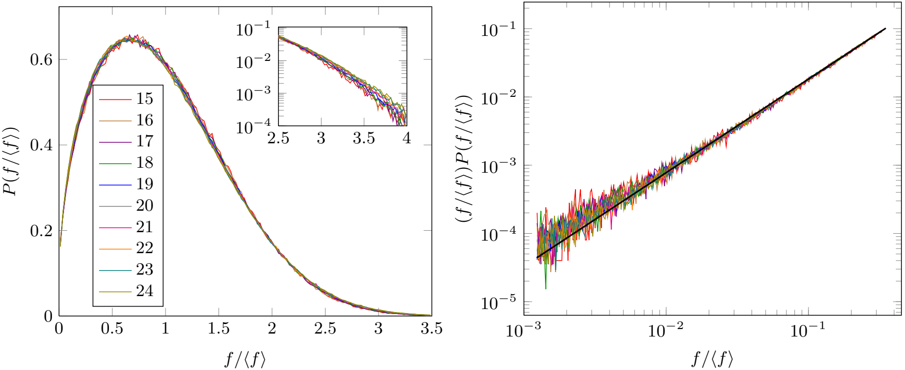



$$g(r) \sim (r-1)^{-\gamma}$$
$$Z(r) \sim d(d+1) + A_d (r-1)^{1-\gamma}$$
$$\gamma = 0.314 \pm 0.004$$

*K, Marcotte, & Torquato, Phys. Rev. E 88, 062151 (2013)*

# Contact force distribution




$$P(f) \sim f^{\theta}$$
$$\theta = 0.371 \pm 0.010$$

*K, Marcotte, & Torquato, Phys. Rev. E 88, 062151 (2013)*