# Numerical search methods for dense sphere packings in higher dimensions

Yoav Kallus

Santa Fe Institute

Jan 11, 2017



## Asymptotic density at 1/p = 0 for

$$d \to \infty$$

$$\phi_{th} \sim d2^{-d}$$

With more patience,  $\phi_{GCP} \sim d \log(d) 2^{-d}$ .

But with unbounded patience, at any d, equilibrium should give  $\phi_{\rm opt}$ , which scales. . .

## Asymptotic density at 1/p = 0 for

$$d \to \infty$$

$$\phi_{th} \sim d2^{-d}$$

With more patience,  $\phi_{GCP} \sim d \log(d) 2^{-d}$ .

But with unbounded patience, at any d, equilibrium should give  $\phi_{\text{opt}}$ , which scales...how?

# Asymptotic density at 1/p=0 for

$$d \rightarrow \infty$$

$$\phi_{th} \sim d2^{-d}$$

With more patience,  $\phi_{GCP} \sim d \log(d) 2^{-d}$ .

But with unbounded patience, at any d, equilibrium should give  $\phi_{\text{opt}}$ , which scales...how?

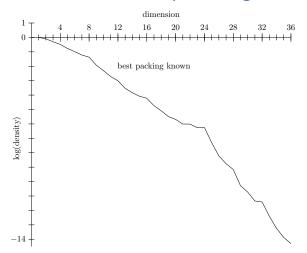
Minkowski:  $\phi_{\rm opt} \gtrsim 2^{-d}$ 

Others:  $\phi_{\sf opt} \gtrsim d2^{-d}$  for all d, and

 $\phi_{\mathrm{opt}} \gtrsim d \log(\log d) 2^{-d}$  for some subseq.  $d \to \infty$ .

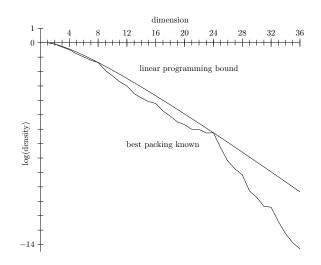
Kabatiansky–Levenshtein:  $\phi_{\text{opt}} \lesssim 2^{-0.5990d}$ 

## Densest known packing for $d \leq 36$

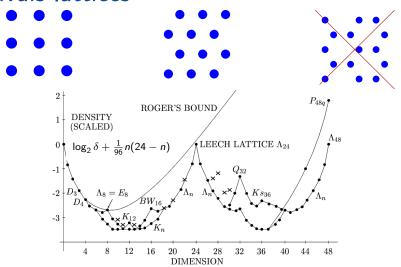


Recently solved in d = 8,24, still open for all other d > 3.

## Densest known packing for $d \leq 36$

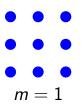


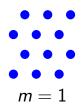
### Bravais lattices

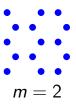


Bravais lattice is densest known packing in 26 out of first 36 dimensions.

# Packings with fixed number of translational orbits







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

## 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 > 1 if  $\mathbf{n}^T G\mathbf{n} \geq 2$  for all  $\mathbf{n} \in \mathbb{Z}^d$ . det G is quasiconcave.

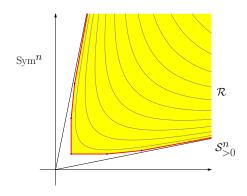
Also, invariant under  $G \mapsto UGU^T$  when  $U \in GL_n(\mathbb{Z})$ .

#### 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
```

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

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

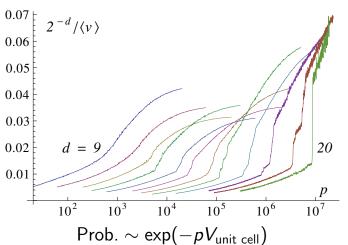


is nonlinear. Nevertheless, can prove, all local optima live on edges.

## Results of enumeration (m = 2)

dimension	3	4	5
# verts.	4	10	34
# rank- $d$ pts. on edges	3 (1)	7 (3)	31+full edge (23)
# locally opt.	3 (1)	7 (3)	29 (20)
degen. of global opt.	3 (1)	2 (0)	5 (2)

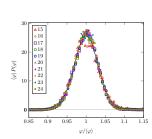
## Thermodynamically sampling lattices

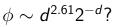


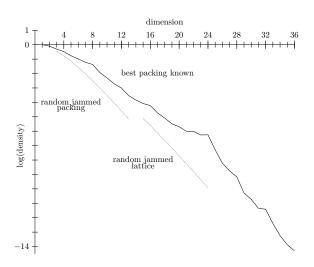
Densest known lattice recovered in some runs for  $d \leq 20$ 

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

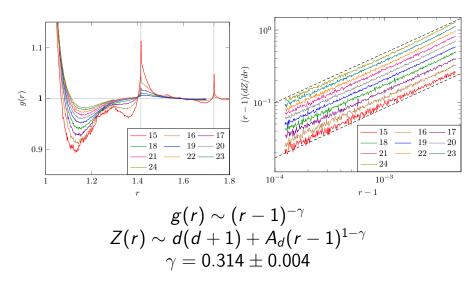
#### Lattice RCP





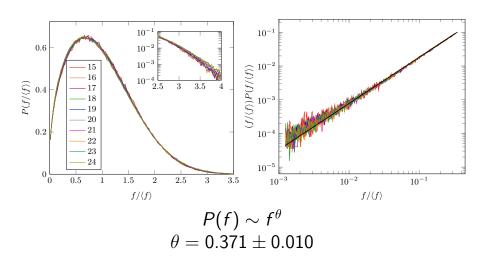


## Pair correlations and quasicontacts



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

#### Contact force distribution



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

#### **Future**

- Cleverer annealing: got  $d \le 22$ ; d = 23 almost working.
- Full enumeration for higher *d*, *m*.
- Annealing for m > 1 (hope to discover packings denser than already known in some d).