Random packing lattices

or: Bravais New World

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Unifying concepts in glass physics VI
Aspen Center for Physics
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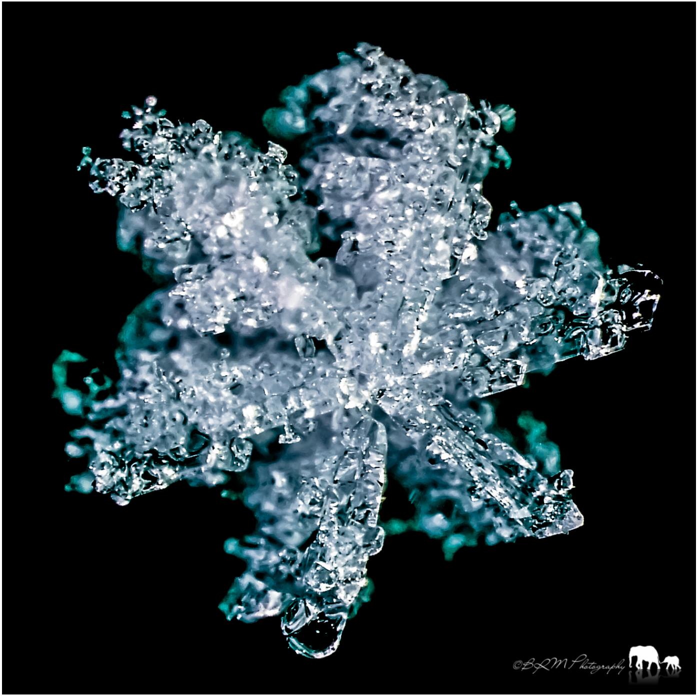
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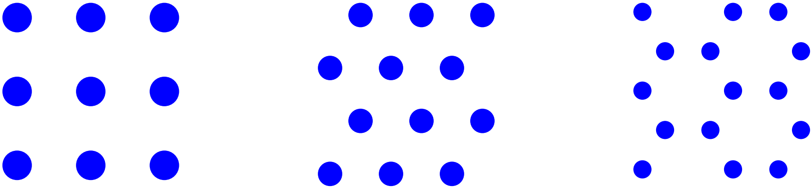
What do I mean by a lattice

$$L = A\mathbb{Z}^n = \{\sum_{i=1}^{n} m_i \mathbf{a}_i : m_i \in \mathbb{Z}\}$$



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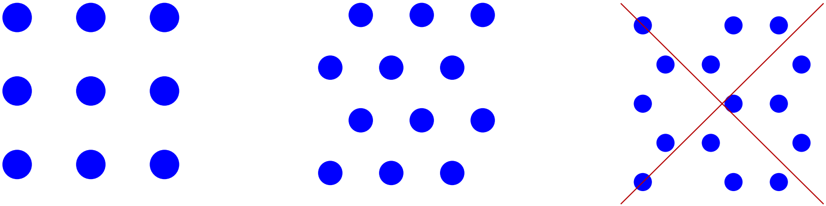

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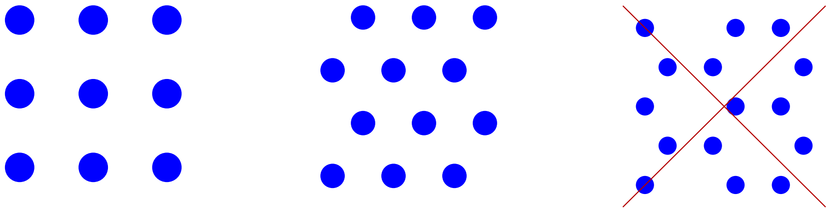
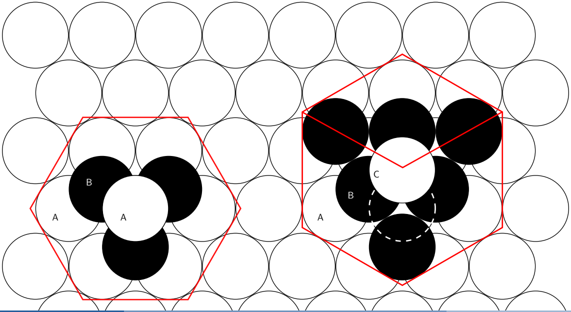
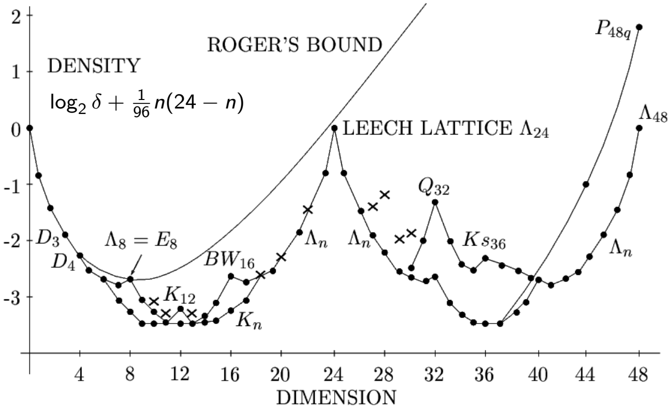
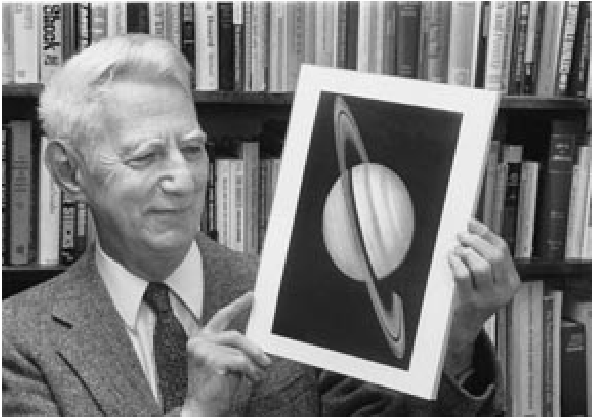




Good packings are often lattices



Why we care about sphere packings in high d?



Packing problem restricted to lattices

Restricted to lattices, what is the densest packing structure?

n	L	
2	A_2	Lagrange (1773)
3	$D_3 = A_3$	Gauss (1840)
4	D_4	Korkin & Zolotarev (1877)
5	D_5	Korkin & Zolotarev (1877)
6	E_6	Blichfeldt (1935)
7	E_7	Blichfeldt (1935)
8	E_8	Blichfeldt (1935)
24	Λ_{24}	Cohn & Kumar (2004)

The space of lattices

Recall: $L = A\mathbb{Z}^n$

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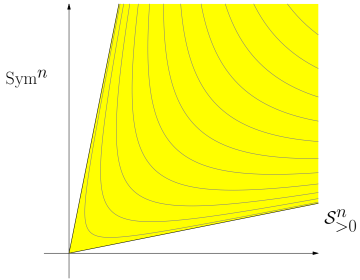
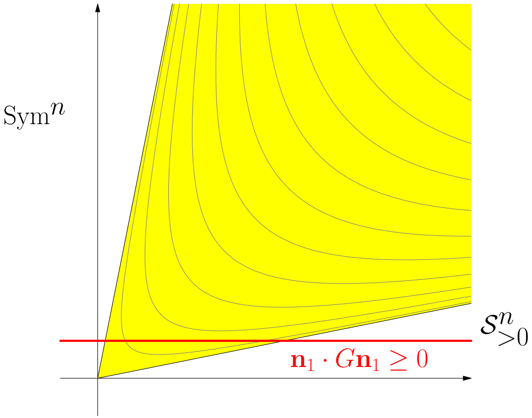
$O(n)\backslash GL_n(\mathbb{R}) = \mathcal{S}^n_{>0} \subset \mathrm{Sym}^n$, the space of symmetric, positive definite matrices: take $G = A^T A$.



The Ryshkov polyhedron

We are interested in the lattices with packing radius ≥ 1:
$\{G \in \mathcal{S}^n_{>0} : \mathbf{n} \cdot G\mathbf{n} \geq 1 \text{ for all } \mathbf{n} \in \mathbb{Z}^n\}$.



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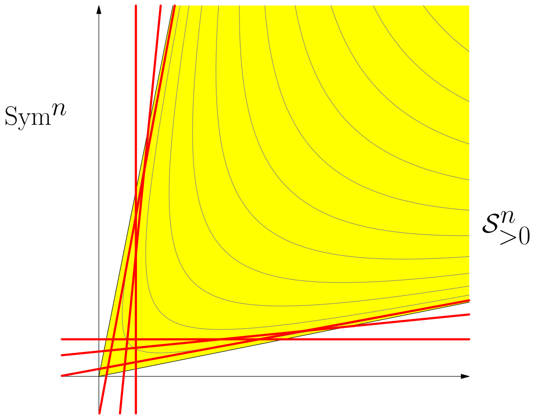

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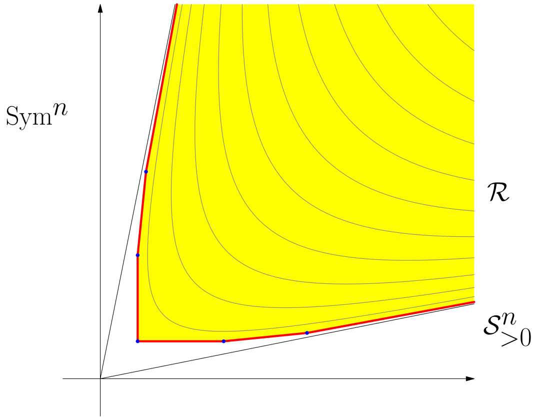

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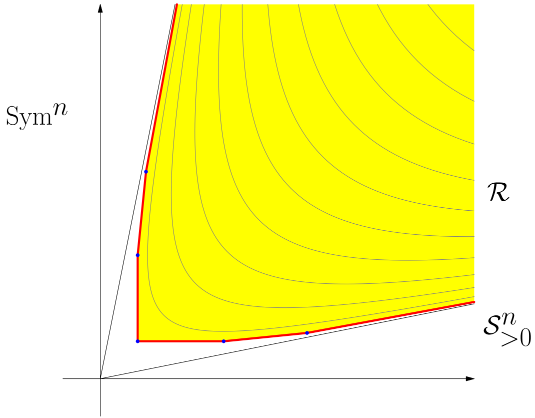
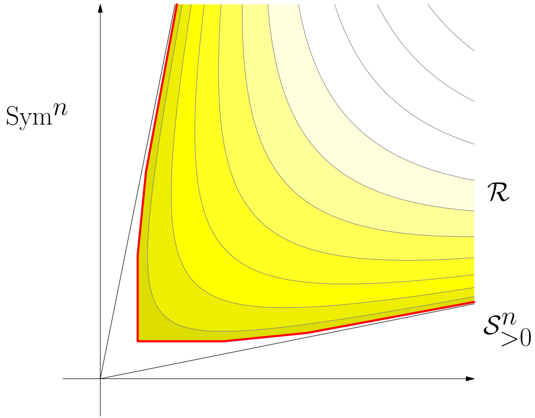
Minimum determinant (maximum density) occurs at vertices, which are finitely enumerable.



The Ryshkov polyhedron

Instead of optimum (zero T), we can ask about finite T:
$P(G) \sim \exp(-\beta p (\det G)^{1/2})$



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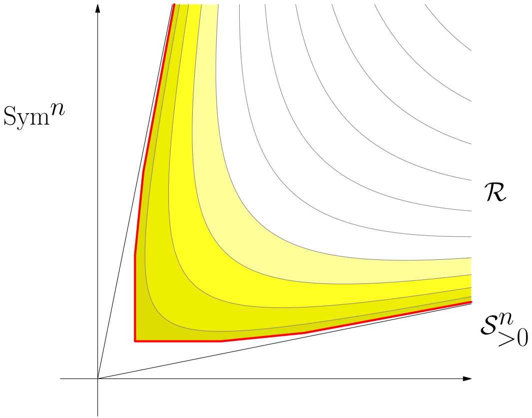
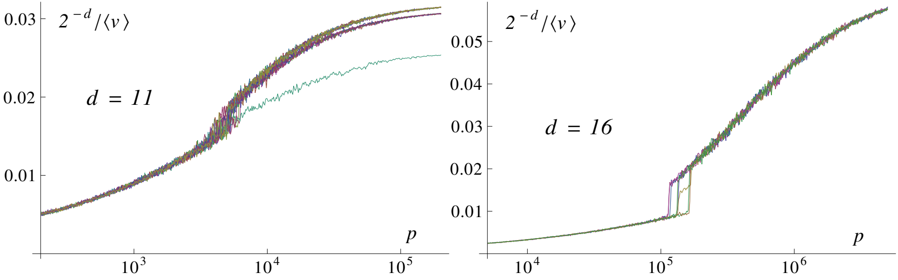


Thermodynamics of hard-sphere lattices



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

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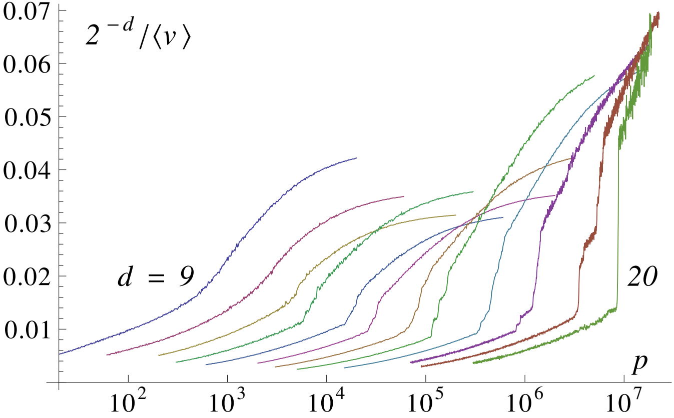

Densest known lattice recovered in some runs for $n \leq 20$

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

A note about symmetry breaking

Is there a symmetry broken in the lattice "freezing" transition?

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$\mathcal{R}$ and det are symmetric under $GL_n(\mathbb{Z})$, and so is the “liquid” state, but not the “solid”.

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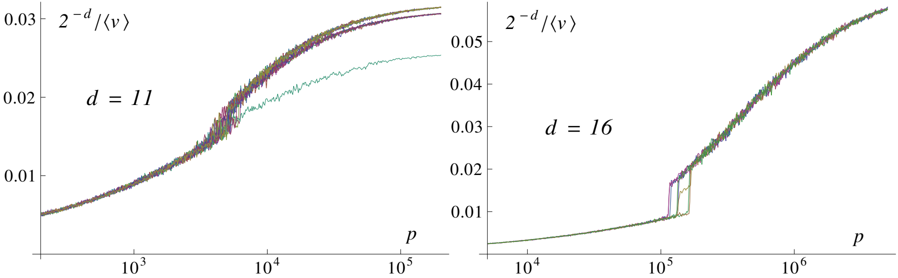

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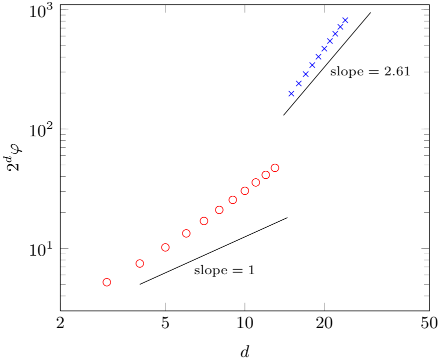
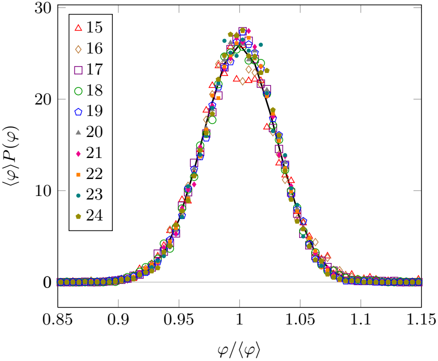
Lattice RCP





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

Lattice isostaticity

Isostaticity:
#constraints = #dof's

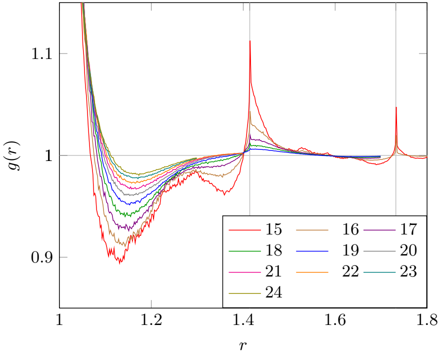
In RCP, Isostaticity $\rightarrow$ average #contacts $= 2d$.

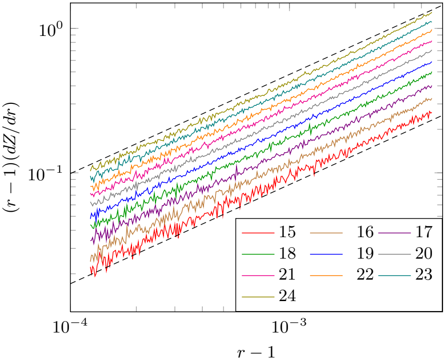
In Lattice RCP: #dof's $= \frac{1}{2}d(d+1)$.
Isostaticity $\rightarrow$ #contacts $= d(d+1)$.

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

d	Runs	Isostatic
13	10,000	365
14	10,000	1,625
15	10,000	5,196
16	10,000	6,761
17	10,000	9,235
18	10,000	9,590
19	20,000	19,200
20	20,000	19,085
21	10,000	9,473
22	10,000	9,406
23	10,000	9,281
24	10,000	9,205

Pair correlations and quasicontacts

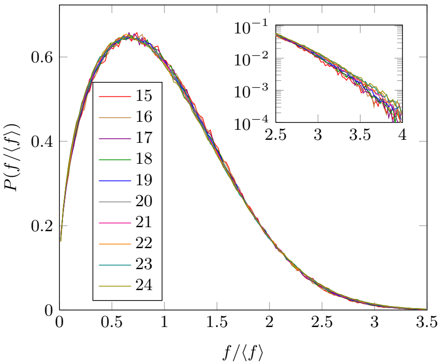


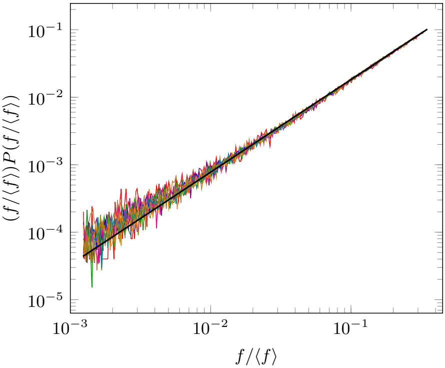


$$g(r) \sim (r-1)^{-\gamma}$$
$$Z(r) \sim d(d+1) + A_d(r-1)^{1-\gamma}$$
$$\gamma = 0.314 \pm 0.004$$

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

Contact force distribution

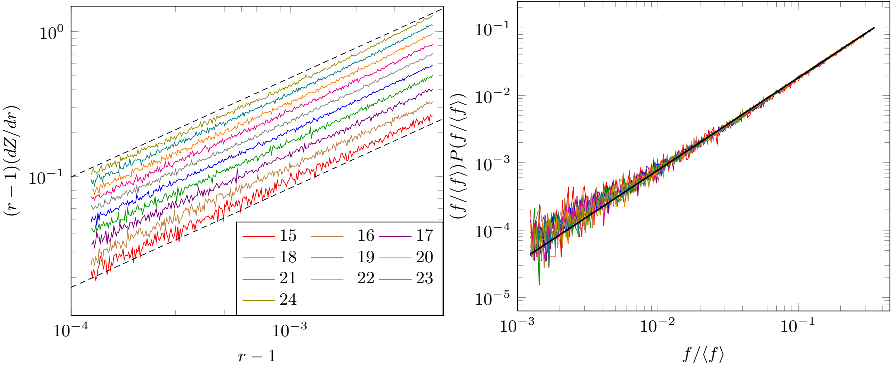




$$P(f) \sim f^{\theta}$$
$$\theta = 0.371 \pm 0.010$$

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

Quasicontacts and weak contacts



$$\gamma = 0.314 \pm 0.004$$
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Uniform sampling of jammed lattices

Extreme lattices can be exhaustively enumerated.

d	2	3	4	5	6	7	8	9
perfect lattices	1	1	2	3	7	33	10916	$>$50000
extreme lattices	1	1	2	3	6	30	2408	$\cdots$

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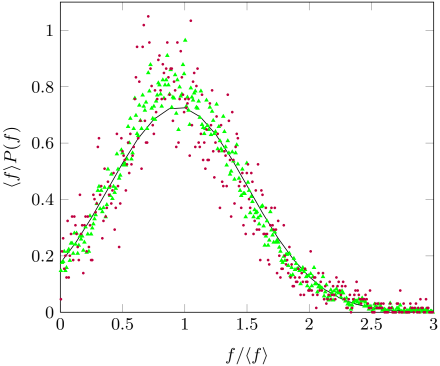
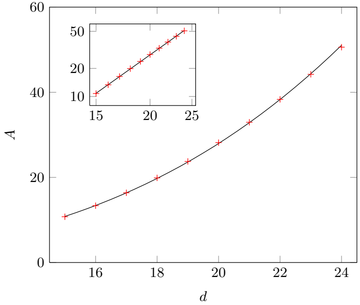


Kallus & Torquato, Phys. Rev. E 90, 022114 (2014)

Quasicontact abundance



$\nu = (1-\gamma)(3+2\theta)/(1+\theta) \approx 3.05$

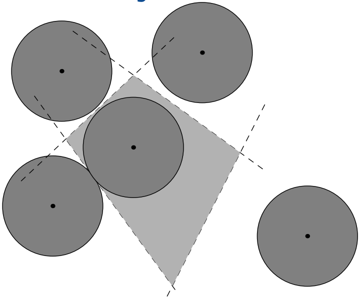
Contacts $\sim d^2$
Quasicontacts $\sim d^\nu$

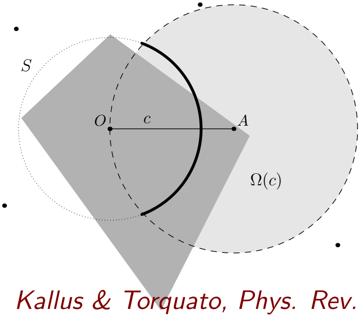
best fit: $A \sim d^{3.30}$

In high-enough dimensions the quasicontact network determines the structure more than the contact network.

Kallus & Torquato, Phys. Rev. E 90, 022114 (2014)

Density estimate from local structure





Using pair correlation:

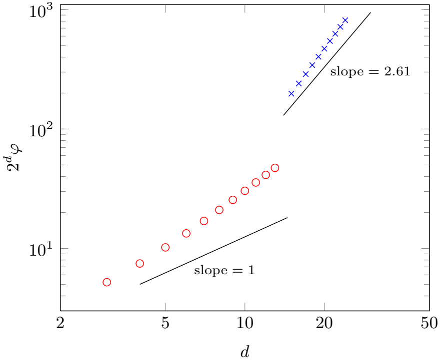
$$g(r) = 1 + \frac{z\delta(r-1)}{\rho S_{d-1}} + \frac{(1-\gamma)A_d(r-1)^{-\gamma}}{\rho S_{d-1} r^{d-1}}$$

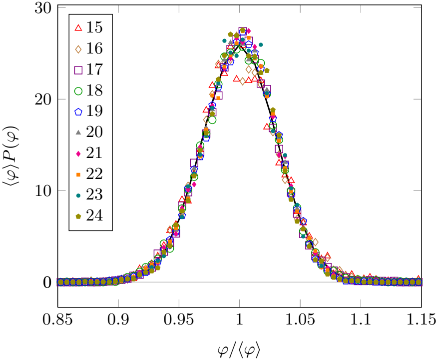
$$g(r) = 0 \text{ for } r < 1$$

	w/o QC	w/ QC
RCP	$2^d\varphi \sim d$	$2^d\varphi \sim d$
LRCP	$2^d\varphi \sim d^2$	$2^d\varphi \sim d^{2.61}$

Kallus & Torquato, Phys. Rev. E 90, 022114 (2014)

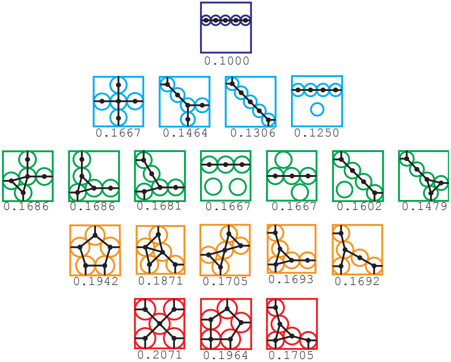
Lattice RCP

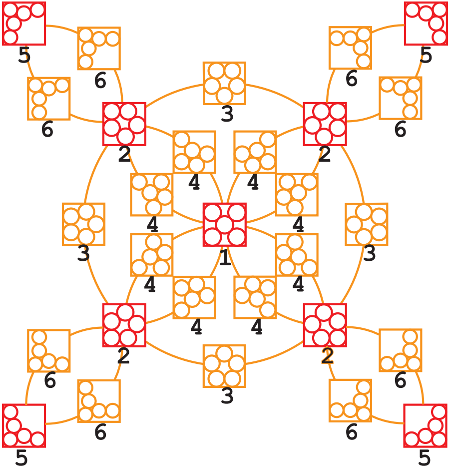




Kallus, Marcotte, & Torquato, Phys. Rev. E 88, 062151 (2013)

Computational topology of config'n space





Carlsson, Gorham, Kahle, & Mason, Phys. Rev. E 85, 011303 (2012)

Conclusions

Lattices in high dimensions have enough dof's to exhibit "disorder".

Lattices are numerically accessible in much higher dimensions than hard-sphere fluids: crystallization for $n \leq 20$, jamming for even larger n.

Random close packed lattices are much denser than RCP hard spheres in n dimensions.

Mathematical structure allows complete enumeration, cell decomposition of config space, contacts$\rightarrow$structure is a linear problem.