Amorphous regular lattices

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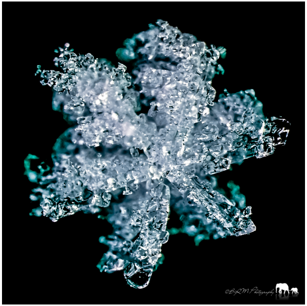
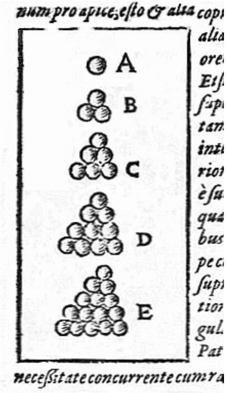


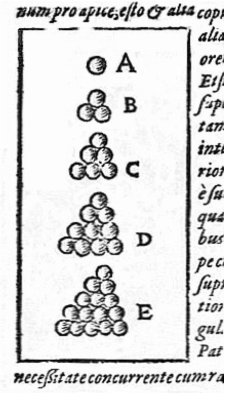
Sphere packing in $\mathbb{R}^3$



Conjecture (Kepler, 1611)

Every nonoverlapping arrangement of congruent spheres in $\mathbb{R}^3$ fills at most $\pi/\sqrt{18} = 0.7404\ldots$ of space.

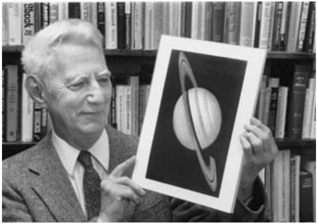
Sphere packing in $\mathbb{R}^3$



Theorem (Hales, 2005)

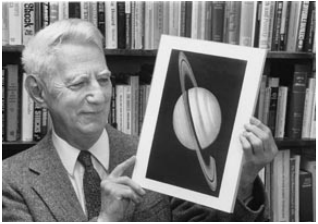
Every nonoverlapping arrangement of congruent spheres in $\mathbb{R}^3$ fills at most $\pi/\sqrt{18} = 0.7404\ldots$ of space.

Sphere packing in $\mathbb{R}^n$



Applications in transmitting, storing, and digitizing signals.

Sphere packing in $\mathbb{R}^n$



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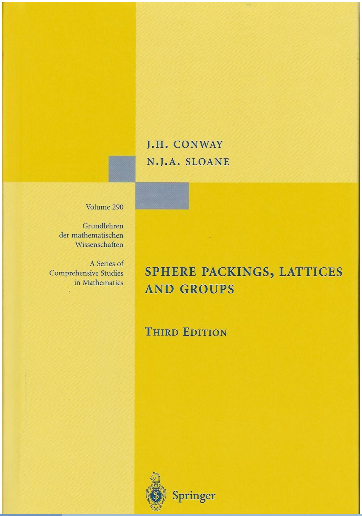
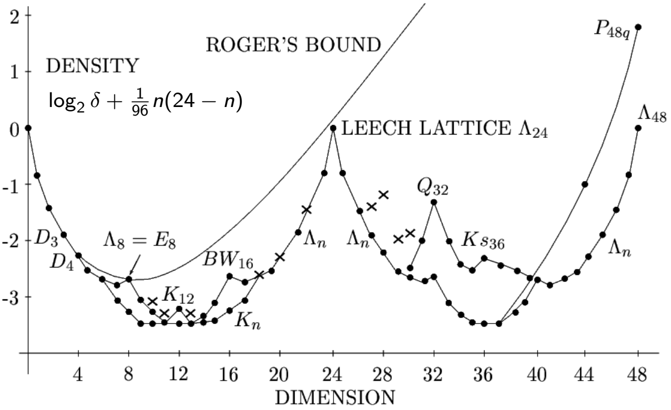


Optimal packing arrangements are often related to exceptional objects from algebra.

Good packings are often lattices



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

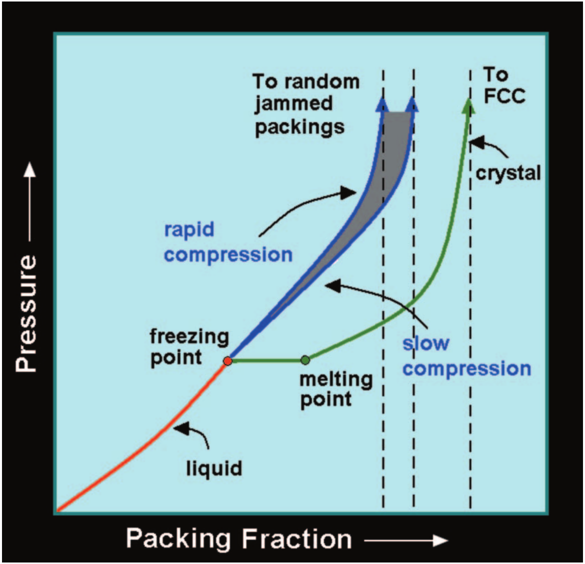
minimize $\det(L)$ subj. to $||\mathbf{x}|| \geq 1$ for all $\mathbf{l} \in L \setminus \{0\}$

Lattices as a special case of packing

Restricted to lattices, what is the densest packing?
(Applications in the geometry of numbers)

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)

Thermodynamics of hard spheres



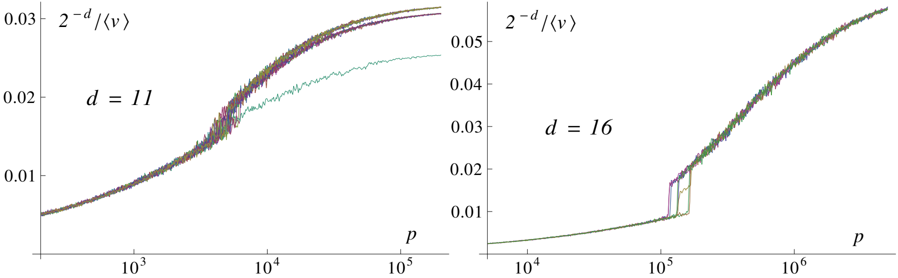
$$U(\mathbf{r}_1, \mathbf{r}_2) = \begin{cases} 0 & \|\mathbf{r}_1 - \mathbf{r}_2\| < 1 \\ \infty & \text{otherwise} \end{cases}$$

sample configurations of N spheres with $P \sim e^{-\beta(U+pV)}$

Torquato & Stillinger, Rev. Mod. Phys. 82, 2633 (2010)

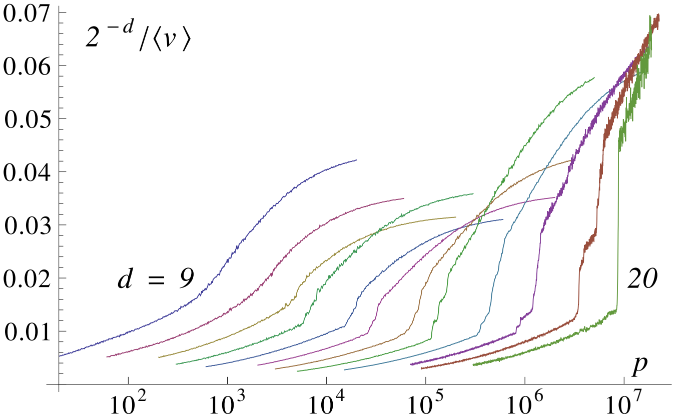
Thermodynamics of hard-sphere lattices

Sample all lattices with $P \sim e^{-\beta(p\,\det(L)+U)}$ where $U = \{0, \infty\}$.



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

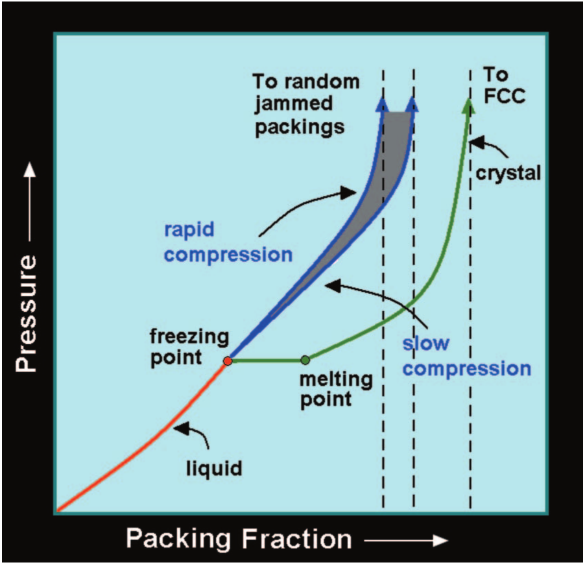
Thermodynamics of hard-sphere lattices



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

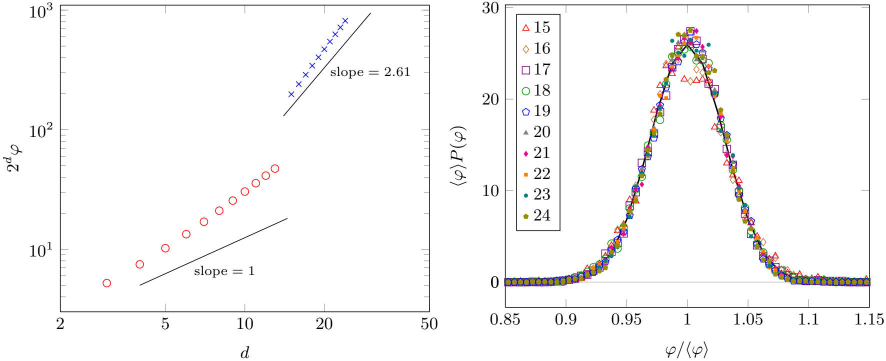
Kallus, Phys. Rev. E 87, 063307 (2013)

Thermodynamics of hard spheres



Torquato & Stillinger, Rev. Mod. Phys. 82, 2633 (2010)

Lattice RCP



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

Lattice isostaticity

Isostaticity:
#constraints = #dof's

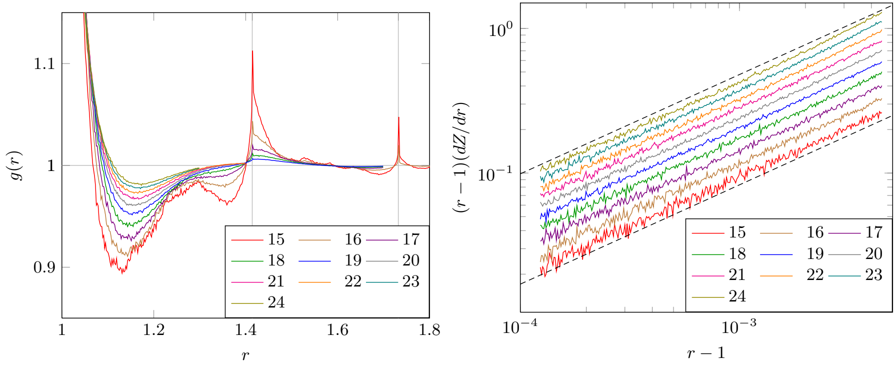
In RCP, Isostaticity $\rightarrow$ average #contacts $= 2d$.

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

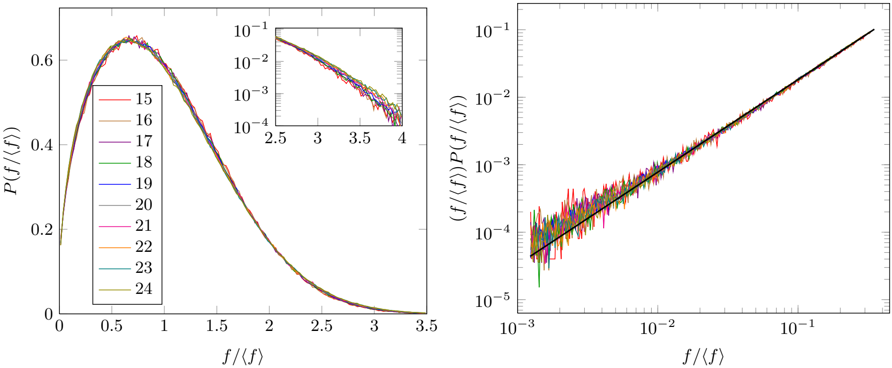
Pair correlations and quasicontacts



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

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

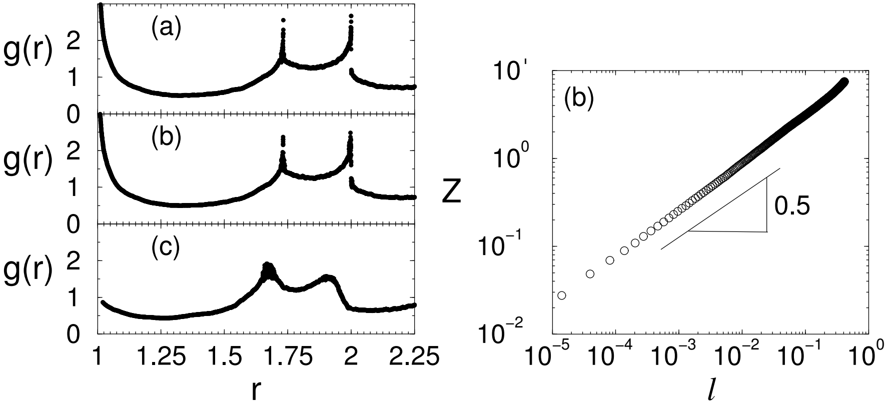
Contact force distribution



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

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

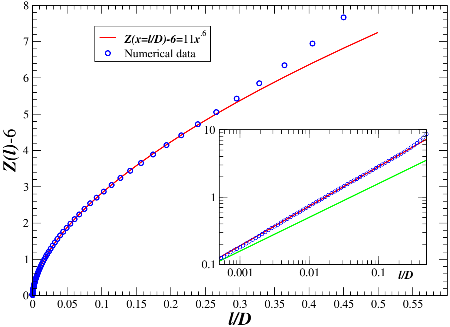
Quasicontacts in RCP

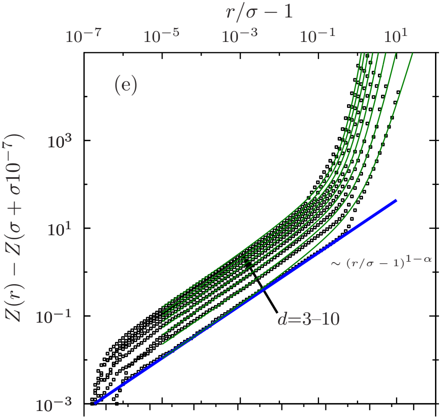


$$\gamma = 0.5?$$

Silbert, Liu, & Nagel, Phys. Rev. E 73, 041304 (2006)

Quasicontacts in RCP

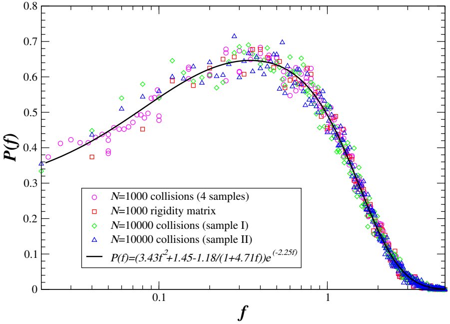


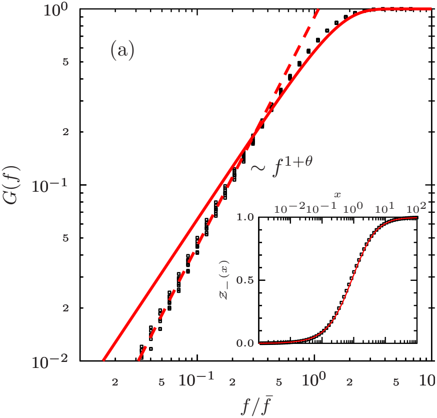


$$\gamma = 0.42 \pm 0.02$$

Donev, Torquato & Stillinger, Phys. Rev. E 71, 011105 (2005)
Charbonneau, Corwin, Parisi, Zamponi, Phys. Rev. Lett. 109, 205501 (2012)

Contact force distribution in RCP

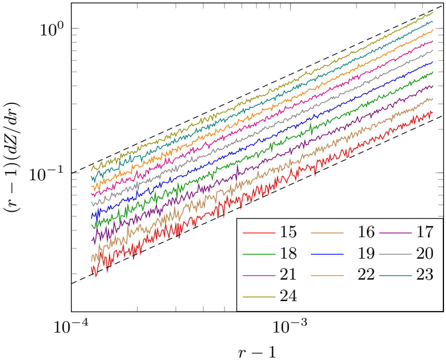


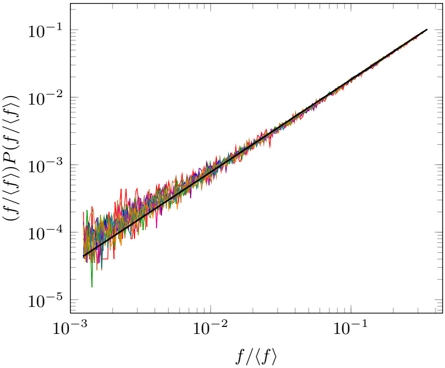


$$P(f) \sim f^{\theta}$$
$$\theta = 0.28 \pm 0.03$$

Donev, Torquato & Stillinger, Phys. Rev. E 71, 011105 (2005)
Charbonneau, Corwin, Parisi, Zamponi, Phys. Rev. Lett. 109, 205501 (2012)

Quasicontacts and weak contacts





$$\gamma = 0.314 \pm 0.004$$
$$\theta = 0.371 \pm 0.010$$

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

Power laws are signatures of approach to jamming

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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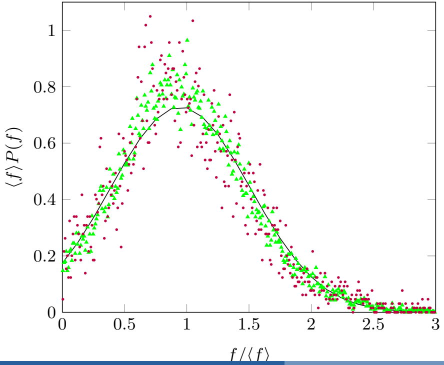
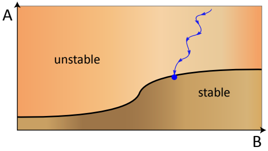
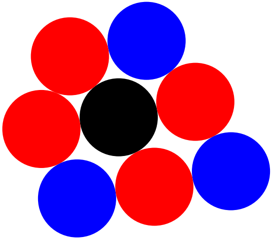


Kallus & Torquato, Phys. Rev. E 90, 0221

Marginal stability





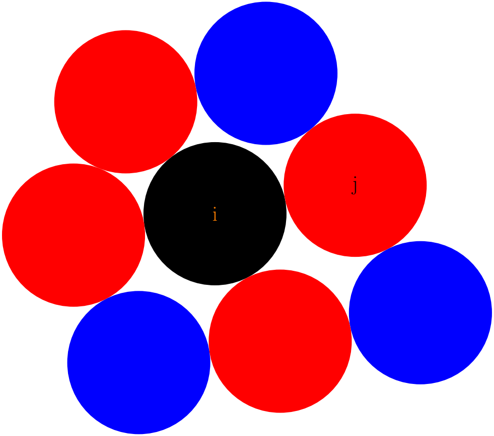
Isostaticity is a manifestation of marginal mechanical stability.

Quasicontacts play no role in mechanical stability.

Instead, they are manifestation of marginal “dynamic” stability.

Contact breaking motion

Due to isostaticity, any contact can be continuously opened by a gap s without disrupting other contacts.



Wyart, Phys. Rev. Lett. 109, 125502 (2012)

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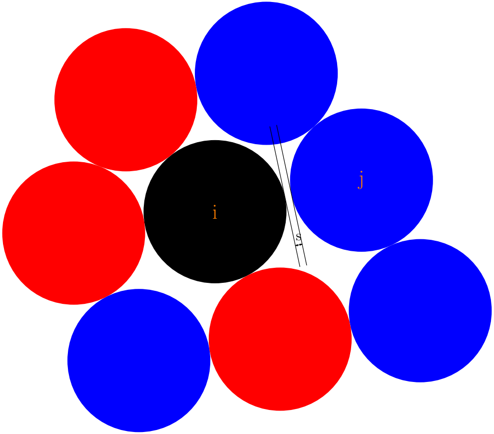

Wyart, Phys. Rev. Lett. 109, 125502 (2012)

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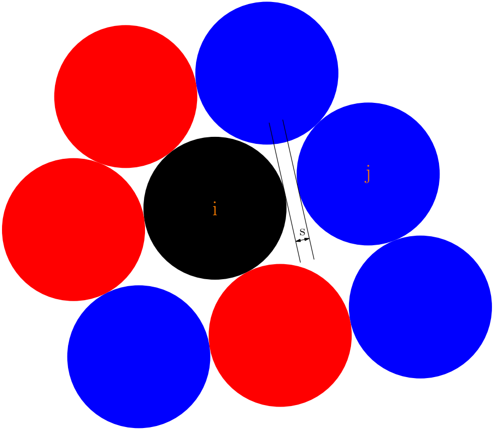

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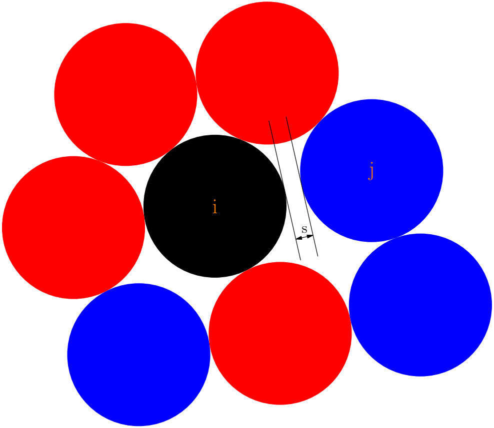

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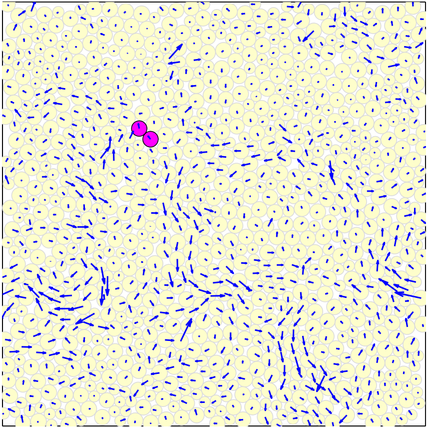
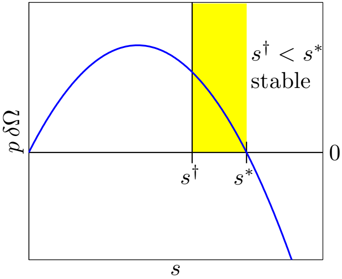


Wyart, Phys. Rev. Lett. 109, 125502 (2012)

Dynamic stability

$$p\delta V(s) = f_{ij}s - C_{ij}s^2 + o(s^2)$$

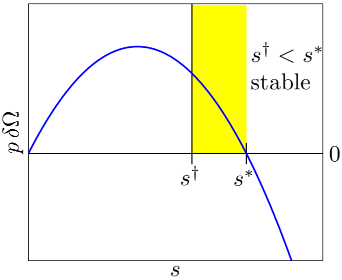


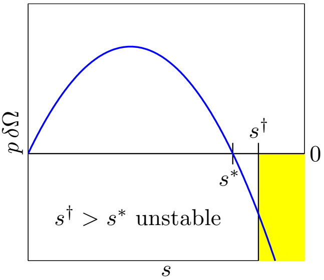
$$s^*_{\min} \sim \frac{f_{\min}}{C} \sim d^{-1/(1+\theta)-2} N^{-1/(1+\theta)-1}$$

$$s^\dagger \sim d^{-\nu/(1-\gamma)} N^{-1/(1-\gamma)}, \text{ where } Z(r) \sim d^\nu (r-1)^{1-\gamma}$$

Dynamic stability

Stability if $s^\dagger \ll s^*_{\min}$



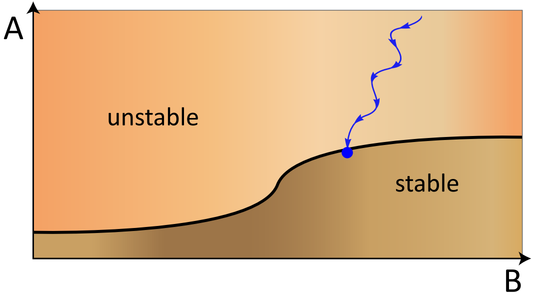


From N-dependence: $\gamma \geq 1/(2+\theta)$

From d-dependence: $\nu \geq (1-\gamma)(3+2\theta)/(1+\theta)$

Marginal dynamic stability

Marginal stability if $s^\dagger \sim s^*_{\mathrm{min}}$

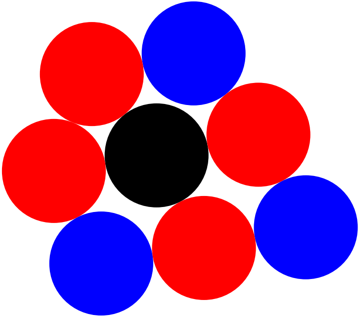


From N-dependence: $\gamma = 1/(2+\theta)$

From d-dependence:
$$\nu = (1-\gamma)(3+2\theta)/(1+\theta) = 2-\gamma$$

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

Quasicontact abundance

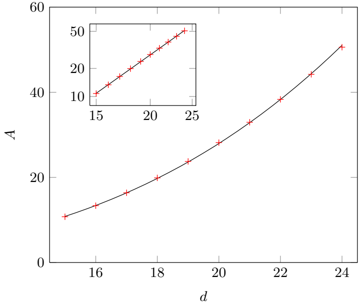


Mean number of contacts in RCP: $2d$

Mean number of quasicontacts: $\sim d^{2-\gamma} \approx d^{1.58}$

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

Marginal dynamic stability in Lattice RCP



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

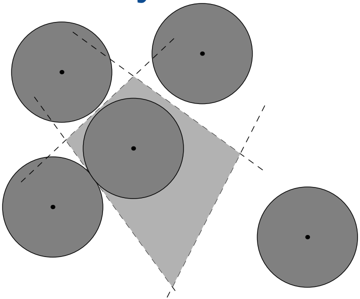
Contacts $\sim d^2$
Quasicontacts $\sim d^\nu$

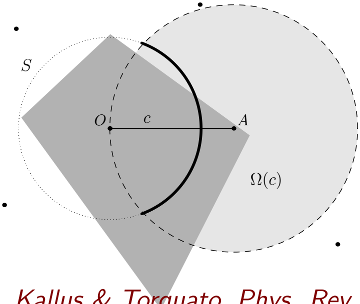
best fit: $A \sim d^{3.30}$

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:

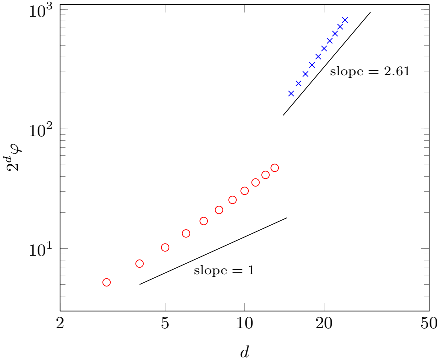
$$g(r) = 1 + \frac{(1-\gamma)A_d(r-1)^{-\gamma}}{\rho S_{d-1} r^{d-1}} + \frac{z\delta(r-1)}{\rho S_{d-1}}$$

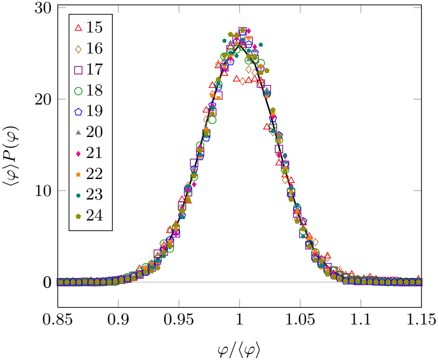
$$g(r) = 0 \text{ for } r < 1$$

	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)

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.

Quasicontacts/weak contact suppression are signatures of approach to jamming, inherently non-equilibrium, and affect structure.