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Workshop on Sphere Packing and Amorphous Materials

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Sphere Packings, Density Fluctuations, Coverings and Quantizers

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Four Different Problems: Interplay Between Geometry and Physics

1. Sphere Packing Problem
   - Applications: low-temperature states of matter (liquids, crystals and glasses), granular media, biological media, communications, string theory, etc.
2. Number Variance Problem
   - Applications: equilibrium and nonequilibrium systems; critical-point phenomena, number theory, hyperuniformity, etc.
3. Covering Problem
   - Applications: wireless communication network layouts, search of high-dimensional data parameter spaces, stereotactic radiation therapy, etc.
4. Quantizer Problem
   - Applications: computer science (e.g., data compression), digital communications, coding and cryptography, optimal meshing of space for numerical applications, etc.

Interaction Energies of Many-Particle Systems

- **Total potential energy** $\Phi_N(\mathbf{r}^N)$ of N identical particles with positions $\mathbf{r}^N \equiv \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N$ in some large volume in d-dimensional Euclidean space $\mathbb{R}^d$ can be resolved into one-body, two-body, . . . , N-body contributions:

$$\Phi_N(\mathbf{r}^N) = \sum_{i=1}^{N} u_1(\mathbf{r}_i) + \sum_{i<j}^{N} u_2(\mathbf{r}_i, \mathbf{r}_j) + \sum_{i<j<k}^{N} u_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \cdots + u_N(\mathbf{r}^N),$$

- To make the statistical-mechanical problem more tractable, this exact many-body potential is often replaced by a mathematically simpler form, e.g., **pairwise interactions**:

$$\Phi_N(\mathbf{r}^N) = \sum_{i<j}^{N} u_2(\mathbf{r}_i, \mathbf{r}_j).$$

- An outstanding problem in classical statistical mechanics is the determination of the **ground states** of $\Phi_N(\mathbf{r}^N)$, which are those configurations that **globally minimize** $\Phi_N(\mathbf{r}^N)/N$.
- More generally, the collection of the **energy minima** (local and global), i.e., **“inherent structures,”** are of great interest.

Reformulations of the Covering and Quantizer Problems

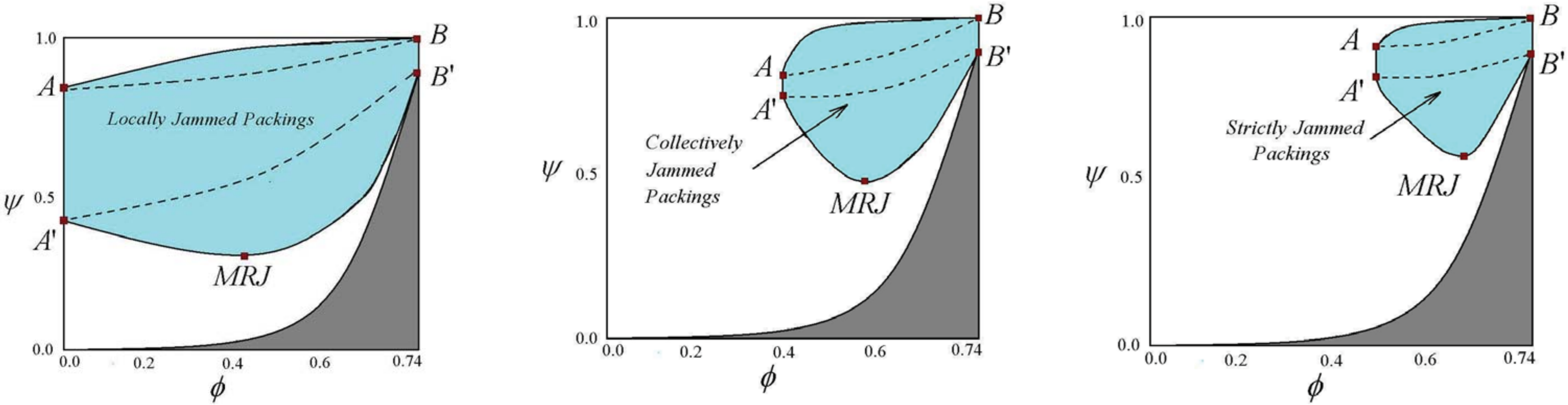
S. Torquato, Physical Review E, 82, 056109 (2010).

- Covering and quantizer problems are reformulated as the determination of the ground states of interacting particles in $\mathbb{R}^d$ that generally involve single-body, two-body, three-body, and higher-body interactions.
- These reformulations allow one now to employ optimization and statistical-mechanical techniques to analyze and solve these ground-state problems.
- This sheds new light on the relationships between the packing, number variance, covering and quantizer problems.
- Results could have applications to the detection of gravitational waves.

Outline

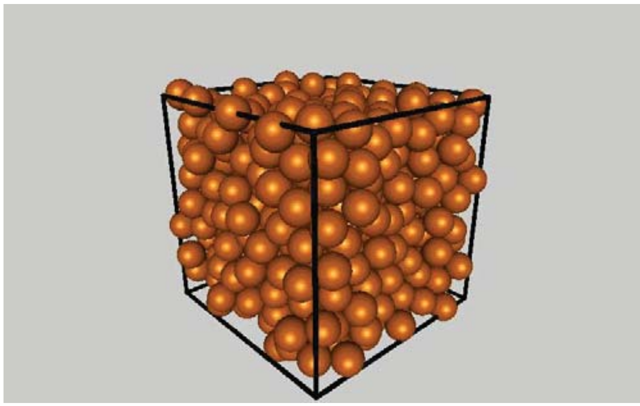
- Diversity of jammed sphere packings in low dimensions
- Review of the packing, number variance, covering and quantizer problems
- Reformulations of the covering and quantizer problems
- Disordered packings yield good coverings and quantizers.

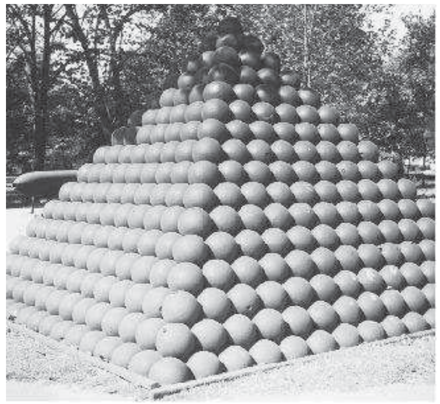
Order Maps for Jammed Sphere Packings



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

Optimal 3D Strictly Jammed Packings



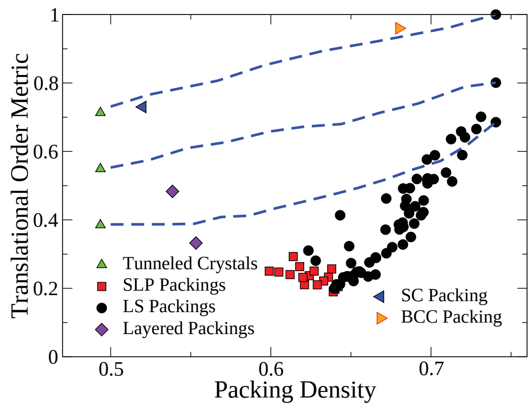


A: $Z = 7$ **MRJ:** $Z = 6$ (**isostatic**) **B:** $Z = 12$

Generating a Diverse Class of Jammed Sphere Packings via Linear Programm

S. Torquato and Y. Jiao, PRE 82, 061302 (2010).

- Solve the adaptive-shrinking cell (ASC) optimization problem, in which the negative of the density is the objective function, using sequential LP methods.
- Produce jammed sphere packings for $d = 2 - 6$ with a diversity of disorder and densities up to the maximal densities.
- A novel feature of this deterministic algorithm is that it can produce a broad range of inherent structures (locally maximally dense and mechanically stable packings), besides the usual disordered ones (MRJ state) and ordered states, with very small computational cost compared to best known algorithms.
- For $d = 3$, can produce with high probability a variety of strictly jammed packings with a packing density anywhere in the wide range $[0.6, 0.7408\ldots]$.

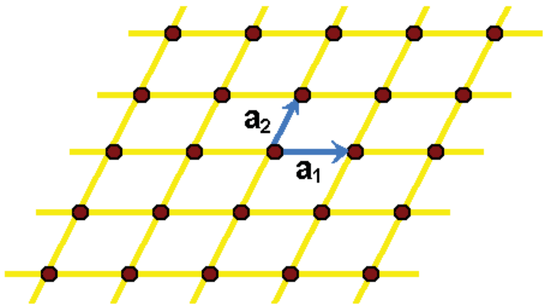


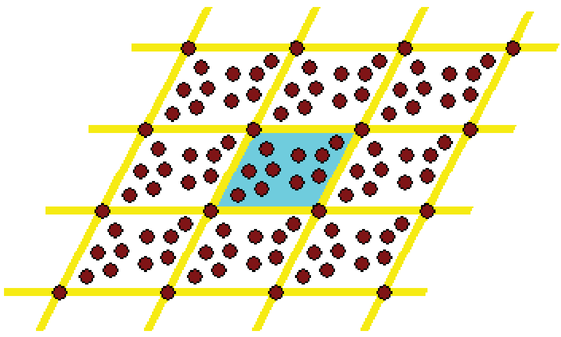
Definitions

- A point process in d-dimensional Euclidean space $\mathbb{R}^d$ is a distribution of an an infinite number of points in $\mathbb{R}^d$ at number density ρ (number of points per unit volume) with configuration $\mathbf{r}_1, \mathbf{r}_2, \ldots$. This is statistically characterized by the n-particle correlation function $g_n(\mathbf{r}_1, \ldots, \mathbf{r}_n)$.
- A lattice Λ in d-dimensional Euclidean space $\mathbb{R}^d$ is the set of points that are integer linear combinations of d basis (linearly independent) vectors $\mathbf{a}_i$, i.e.,

$$\{n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + \cdots + n_d\mathbf{a}_d \mid n_1, \ldots, n_d \in Z\}$$

  The space $\mathbb{R}^d$ can be geometrically divided into identical regions F called fundamental cells, each of which contains just one point. For example, in $\mathbb{R}^2$:





- Every lattice has a dual (or reciprocal) lattice Λ^*.
- A periodic point distribution in $\mathbb{R}^d$ is a fixed but arbitrary configuration of N points ($N \geq 1$) in each fundamental cell of a lattice.

Voronoi cells in $\mathbb{R}^d$

- Associated with each point $\mathbf{r}_i \in \mathcal{P}$ is its Voronoi cell, $\mathcal{V}(\mathbf{r}_i)$, which is defined to be the region of space nearer to the point at $\mathbf{r}_i$ than to any other point $\mathbf{r}_j$.
- A deep hole in a lattice Λ is one whose distance to a lattice point is a global maximum. The distance $\mathcal{R}_c$ to the deepest hole of a lattice is the covering radius and is equal to the circumradius of the associated Voronoi cell (the radius of the smallest circumscribed sphere).

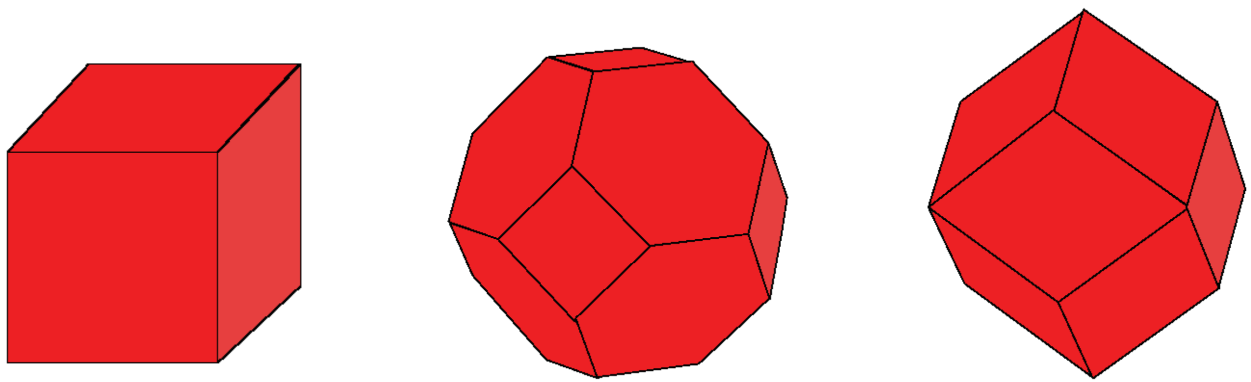


Figure 1: Voronoi cells in $\mathbb{R}^3$ for simple cubic ($\mathbb{Z}^3 \equiv \mathbb{Z}^3_*$), body-centered cubic ($A_3^* \equiv D_3^*$), and face-centered cubic ($A_3 \equiv D_3$) lattices are the cube (left), truncated octahedron (middle), and rhombic dodecahedron (right).

Sphere Packing Problem

- **The packing density ϕ is the fraction of space $\mathbb{R}^d$ covered by identical nonverlapping (hard) spheres of unit diameter, i.e.,**

$$\phi = \rho v_1(1/2),$$

where

$$v_1(R) = \frac{\pi^{d/2} R^d}{\Gamma(1 + d/2)},$$

is the volume of a d-dimensional sphere of radius R.

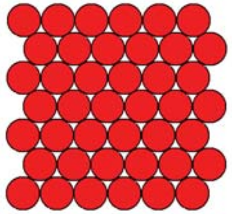
- **The sphere packing problem:**
Among all packings of congruent spheres in $\mathbb{R}^d$, what is the maximal density $\phi_{\max}$ and what are the corresponding arrangements of the spheres?

- **It is well known that the sphere packing problem can be posed as an energy minimization problem involving certain pairwise interactions between points in $\mathbb{R}^d$, e.g.,**

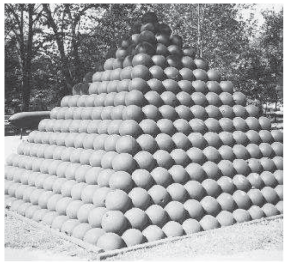
$$\lim_{M \to \infty} \frac{1}{N} \sum_{i<j}^{N} \frac{1}{|\mathbf{r}_{ij}|^M} \qquad \textbf{(Riesz potential)}$$

Sphere Packing Problem

- For $d = 2$, triangular lattice: $\phi_{\text{max}} = \pi/\sqrt{12} \approx 0.91$ (Fejes Tóth, 1940).



- For $d = 3$, Kepler (1606) conjectured that optimal packing is FCC lattice: $\phi_{\text{max}} = \pi/\sqrt{18} \approx 0.74$ (Hales 1998, 2005).



- Each dimension has its own distinct properties.
- In certain sufficiently low dimensions, optimal packings are believed to be lattice packings. Certain dimensions are amazingly symmetric and dense: $d = 8$ (E_8 lattice) and $d = 24$ (Leech lattice) (Cohn & Kumar, 2009).
- Finding shortest lattice vector for a lattice grows superexponentially with d.
- In $\mathbb{R}^{10}$, the best known arrangement is a non-lattice packing.
- In high d, densest packings could be disordered (Torquato & Stillinger, 2006; Scardicchio et al., 2008; Zachary & Torquato, 2011). Link to Cohn-Elkies (2003)

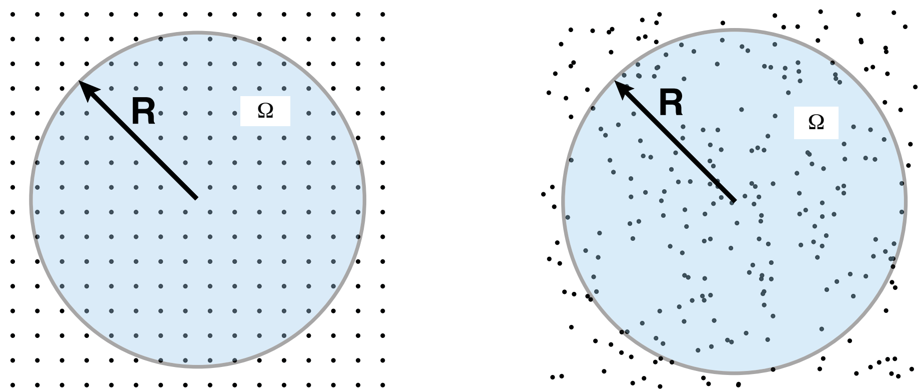
Table 1: Best known solutions to the sphere packing problem in selected dimensions; see Conway and Sloane (1998) for details.

Dimension, d	Packing	Packing density, ϕ
1	$A_1^* = \mathbb{Z}$	1
2	$A_2^* \equiv A_2$	$\pi/\sqrt{12} = 0.906899\ldots$
3	$A_3 \equiv D_3$	$\pi/\sqrt{18} = 0.740480\ldots$
4	$D_4 \equiv D_4^*$	$\pi^2/16 = 0.616850\ldots$
5	D_5	$2\pi^2/(30\sqrt{2}) = 0.465257\ldots$
6	E_6	$3\pi^3/(144\sqrt{3}) = 0.372947\ldots$
7	E_7	$\pi^3/105 = 0.295297\ldots$
8	$E_8 = E_8^*$	$\pi^4/384 = 0.253669\ldots$
9	Λ_9	$\sqrt{2}\pi^4/945 = 0.145774\ldots$
10	P_{10c}	$\pi^5/3072 = 0.099615\ldots$
12	Λ_{12}^{max}	$\pi^6/23040 = 0.041726\ldots$
16	Λ_{16}	$\pi^8/645120 = 0.014708\ldots$
24	$\Lambda_{24} = \Lambda_{24}^*$	$\pi^{24}/479001600 = 0.001929\ldots$

Local Density Fluctuations for General Point Patterns

Torquato and Stillinger, PRE (2003)

- Points can represent molecules of a material, stars in a galaxy, or trees in a forest. Let Ω represent a spherical window of radius R in d-dimensional Euclidean space $\mathbb{R}^d$.



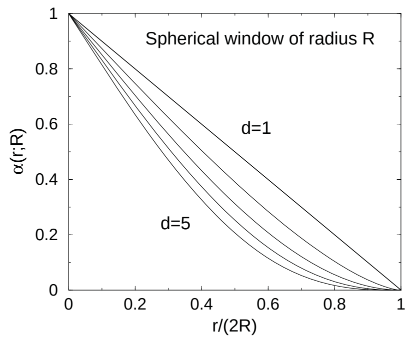
- Denote by $\sigma^2(R) \equiv \langle N^2(R)\rangle - \langle N(R)\rangle^2$ the number variance.
- For a Poisson point pattern and many correlated point patterns, $\sigma^2(R) \sim R^d$.
- We call point patterns whose variance grows more slowly than R^d hyperuniform (infinite-wavelength fluctuation vanish). This implies that structure factor $S(k) \to 0$ for $k \to 0$.
- All crystals and quasicrystals are hyperuniform such that $\sigma^2(R) \sim R^{d-1}$ – number variance grows like window surface area.
- The hyperuniformity concept enables us to classify crystals and quasicrystals with special disordered point processes.

Number Variance Problem

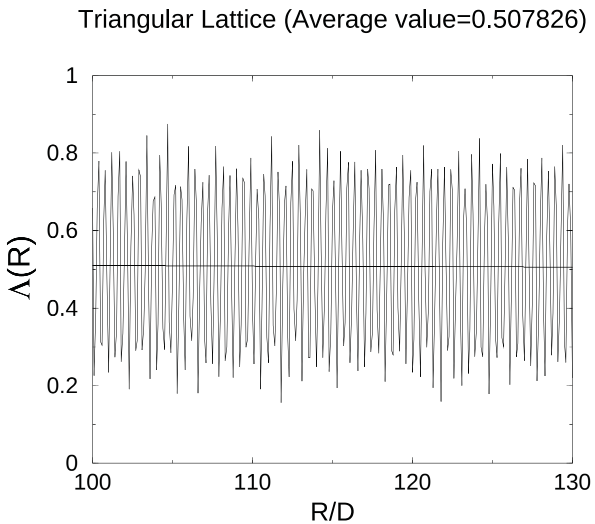
- **We showed**

$$\sigma^2(R) = 2^d\phi\left(\frac{R}{D}\right)^d\left[1 - 2^d\phi\left(\frac{R}{D}\right)^d + \frac{1}{N}\sum_{i\neq j}^{N}\alpha(r_{ij};R)\right]$$

where $\alpha(r;R)$ is scaled intersection volume of 2 windows separated by r, which can be viewed as a repulsive pair potential:



- **Finding global minimum of $\sigma^2(R)$ equivalent to finding ground state.**



Hyperuniformity and Number Theory

- Useful way to categorize crystals, quasicrystals and special disordered point patterns.

2D Pattern	$\overline{\Lambda}/\phi^{1/2}$
Triangular Lattice	0.508347
Square Lattice	0.516401
Honeycomb Lattice	0.567026
Kagomé Lattice	0.586990
Penrose Tiling	0.597798
Step+Delta-Function g_2	0.600211
Step-Function g_2	0.848826
One-Component Plasma	1.12838

- Every lattice Λ with lattice vector $\mathbf{p}$ has a dual (or reciprocal) lattice Λ^* in which the sites of the lattice are specified by the dual (reciprocal) lattice vector $\mathbf{q}$ such that $\mathbf{q}\cdot\mathbf{p} = 2\pi m$, where $m = \pm 1, \pm 2, \pm 3 \cdots$.
- We showed that for a lattice

$$\sigma^2(R) = \sum_{\mathbf{q}\neq \mathbf{0}} \left(\frac{2\pi R}{q}\right)^d [J_{d/2}(qR)]^2, \qquad \overline{\Lambda} = 2^d \pi^{d-1} \sum_{\mathbf{q}\neq \mathbf{0}} \frac{1}{|\mathbf{q}|^{d+1}}.$$

- Epstein zeta function for a lattice is defined by

$$Z_Q(s) = \sum_{\mathbf{q}\neq \mathbf{0}} \frac{1}{|\mathbf{q}|^{2s}}, \qquad \text{Re } s > d/2.$$

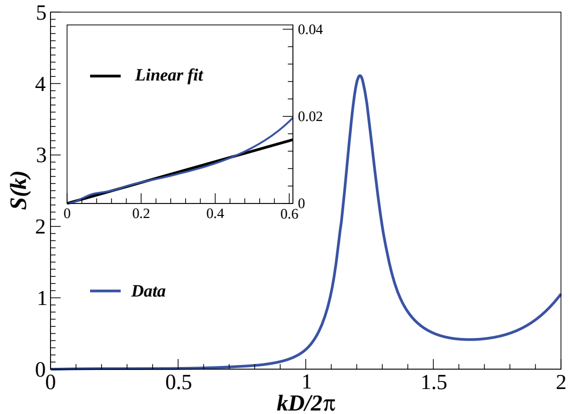
Sarnak and Strömbergsson (2006)

Table 2: Best known solutions to the asymptotic number variance problem in selected dimensions. Values reported for $d = 1, 2$ and 3 and $d = 4-8$ are taken from Torquato & Stillinger (2003) and Zachary & Torquato (2009), respectively. Values reported for $d = 12, 16$ and 24 have been determined in the present work.

Dimension, d	Structure	Scaled $\overline{\Lambda}$
1	$A_1^* = \mathbb{Z}$	0.083333
2	$A_2^* \equiv A_2$	0.12709
3	$A_3^* \equiv D_3^*$	0.15560
4	$D_4^* \equiv D_4$	0.17488
5	Λ_5^{2*}	0.19069
6	E_6^*	0.20221
7	D_7^+	0.21037
8	$E_8^* = E_8$	0.21746
12	$K_{12}^* \equiv K_{12}$	0.24344
16	$\Lambda_{16}^* \equiv \Lambda_{16}$	0.25629
24	$\Lambda_{24}^* = \Lambda_{24}$	0.26775

Hyperuniformity and Jammed Packings

- Conjecture (Torquato & Stillinger, 2003): All strictly jammed saturated sphere packings are hyperuniform.
- 3D MRJ packings of monodisperse spheres have been shown to be hyperuniform with quasi-long-range (QLR) pair correlations with decay $1/r^4$ (Donev, Stillinger & Torquato, PRL, 2005):



- What about other MRJ particle packings, including spheres with a size distribution and nonspherical particles in $\mathbb{R}^d$?
  - Apparently, hyperuniform QLR correlations with decay $1/r^{d+1}$ are a universal feature of general MRJ packings in $\mathbb{R}^d$.
    - Zachary, Jiao and Torquato, PRL (2011): ellipsoids, superballs, sphere mixtures
    - Berthier et al, PRL (2011): sphere mixtures
    - Jiao and Torquato (2011); polyhedra

Covering Problem

- Surround each of the points of a point process $\mathcal{P}$ in $\mathbb{R}^d$ by congruent overlapping spheres of radius R such that the spheres cover the space. The covering density θ is defined as follows:
$$\theta = \rho v_1(R),$$
where $v_1(R)$ is the volume of a d-dimensional sphere of radius R.

- The covering problem asks for the arrangement of points with the least density θ. We define the covering radius $\mathcal{R}_c$ for any configuration of points in $\mathbb{R}^d$ to be the minimal radius of the overlapping spheres to cover $\mathbb{R}^d$.

Figure 2: Coverings of the plane with overlapping circles centered on the triangular lattice ($\theta = 2\pi/(3\sqrt{3}) = 1.2092\ldots$) and the square lattice ($\theta = \pi/2 = 1.5708\ldots$).

Figure 3: Voronoi cells illustrated in two dimensions for the triangular lattice and an irregular point pattern. Left: $\mathcal{R}_c$ equals circumradius of associated Voronoi cell. Right: This is not true; noncongruent Voronoi cells and centroids do not coincide with the points of the point process.

Covering Problem

- The covering density associated with A_d^* at unit number density $\rho = 1$ is known exactly for any dimension d:

$$\theta = v_1(1)\sqrt{d+1}\left[\frac{d(d+2)}{12(d+1)}\right]^{d/2}.$$

- For the hypercubic lattice $\mathbb{Z}^d$ at $\rho = 1$,

$$\theta = v_1(1)\frac{d^{d/2}}{2^d}.$$

- Thus the ratio of the covering density for A_d^* to that of $\mathbb{Z}^d$ is given by

$$\frac{\theta(A_d^*)}{\theta(Z^d)} = \frac{\sqrt{d+1}}{3^{d/2}}\left[\frac{d+2}{d+1}\right]^{d/2}.$$

For large d, this ratio becomes

$$\frac{\theta(A_d^*)}{\theta(Z^d)} \sim \frac{\sqrt{de}}{3^{d/2}}.$$

- Until recently, A_d^* was the best known lattice covering in all dimensions $d \leq 23$. However, for $6 \leq \theta \leq 17$, Schürmann and Vallentin (2006) have discovered other lattice coverings that are slightly thinner than those for A_d^*.

Table 3: Best known solutions to the covering problem in selected dimensions.

Dimension, d	Covering	Covering Density, θ
1	$A_1^* \equiv \mathbb{Z}$	1
2	$A_2^* \equiv A_2$	1.2092
3	$A_3^* \equiv D_3^*$	1.4635
4	A_4^*	1.7655
5	A_5^*	2.1243
6	L_6^{c1}	2.4648
7	L_7^c	2.9000
8	L_8^c	3.1422
9	A_9^5	4.3401
10	A_{10}^*	5.2517
12	A_{12}^*	7.5101
16	A_{16}^*	15.3109
17	A_{17}^*	18.2878
18	A_{18}^*	21.8409
24	Λ_{24}	7.9035

Quantizer Problem

- A d-dimensional quantizer is device that takes as an input a point at position $\mathbf{x}$ in $\mathbb{R}^d$ generated from a uniform distribution and outputs the nearest point $\mathbf{r}_i$ of the point process $\mathcal{P}$ to $\mathbf{x}$.
- Equivalently, if the input $\mathbf{x}$ belongs to the Voronoi cell $\mathcal{V}(\mathbf{r}_i)$, the output is $\mathbf{r}_i$.
- Specifically, the quantizer problem is to choose the N-point configuration so as to minimize the scaled dimensionless error (sometimes called the distortion)

$$\mathcal{G} = \frac{1}{d}\langle R^2 \rangle,$$

where

$$\langle R^2 \rangle = \frac{\displaystyle\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \int_{\mathcal{V}(\mathbf{r}_i)} |\mathbf{x}-\mathbf{r}_i|^2 d\mathbf{x}}{\langle \text{Vol}(\mathcal{V})\rangle^{1+\frac{2}{d}}},$$

$$\langle \text{Vol}(\mathcal{V})\rangle = \left[\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \text{Vol}(\mathcal{V}(\mathbf{r}_i))\right]$$

Figure 4: Any point $\mathbf{x}$ is quantized (“rounded-off”) to the nearest point $\mathbf{r}_i$. Left panel: Triangular lattice. Right panel: Irregular point process.

- The lattice quantizer solution in $\mathbb{R}^d$ reduces to finding the lattice Voronoi polytope with minimal second moment of inertia.

Quantizer Problem

- Best known quantizers in any dimension d are lattices, usually the duals of the densest known packings, except for $d = 9$ and 10 (Agrell & Eriksson, 1998).

Table 4: Best known solutions to the quantizer problem in selected dimensions.

Dimension, d	Quantizer	Scaled Error, $\mathcal{G}$
1	$A_1^* = \mathbb{Z}$	0.083333
2	$A_2^* \equiv A_2$	0.080188
3	$A_3^* \equiv D_3^*$	0.078543
4	$D_4^* \equiv D_4$	0.076603
5	D_5^*	0.075625
6	E_6^*	0.074244
7	E_7^*	0.073116
8	$E_8^* = E_8$	0.071682
9	L_9^{AE}	0.071626
10	D_{10}^+	0.070814
12	$K_{12}^* \equiv K_{12}$	0.070100
16	$\Lambda_{16}^* \equiv \Lambda_{16}$	0.068299
24	$\Lambda_{24}^* = \Lambda_{24}$	0.065771

Table 5: Comparison of the Four Problems

Dimension, d	Quantizer	Covering	Variance	Packing
1	$A_1^* = \mathbb{Z}$	$A_1^* = \mathbb{Z}$	$A_1^* = \mathbb{Z}$	$A_1^* = \mathbb{Z}$
2	$A_2^* \equiv A_2$	$A_2^* \equiv A_2$	$A_2^* \equiv A_2$	$A_2^* \equiv A_2$
3	$A_3^* \equiv D_3^*$	$A_3^* \equiv D_3^*$	$A_3^* \equiv D_3^*$	$A_3 \equiv D_3$
4	$D_4^* \equiv D_4$	A_4^*	$D_4^* \equiv D_4$	$D_4^* \equiv D_4$
5	D_5^*	A_5^*	Λ_5^{2*}	D_5
6	E_6^*	L_6^{c1}	E_6^*	E_6
7	E_7^*	L_7^c	Λ_7^{3*}	E_7
8	E_8	L_8^c	E_8	E_8
9	L_9^{AE}	A_9^5	Λ_9^*	Λ_9
10	D_{10}^+	A_{10}^*	Λ_{10}^*	P_{10c}
12	K_{12}	A_{12}^*	Λ_{12}^{max*}	Λ_{12}^{max}
16	Λ_{16}^*	A_{16}^*	Λ_{16}^*	Λ_{16}
24	Λ_{24}	Λ_{24}	Λ_{24}	Λ_{24}

- **For $d =$1, 2 and 3, the best known solutions for each of the 4 problems are related lattices. However, such relationships may or may not exist for $d \geq 4$, depending on the peculiarities of the dimensions involved.**

Nearest-Neighbor Functions

- We recall the definition of the **"void" nearest-neighbor probability density function** $H_V(R)$:

$$H_V(R)\,dR \quad = \quad \text{Probability that a point of the point process lies at a distance between } R \text{ and } R+dR \text{ from a randomly chosen point in } \mathbb{R}^d.$$

- The **"void" exclusion probability** $E_V(R)$ is the *complementary cumulative distribution function* associated with $H_V(R)$:

$$E_V(R) = \int_R^\infty H_V(x)dx,$$

and hence is a monotonically decreasing function of R. Thus, $E_V(R)$ has the following probabilistic interpretation:

$$E_V(R) \quad = \quad \text{Probability of finding a randomly placed spherical cavity of radius } R \text{ empty of any points.}$$

- There is another interpretation of E_V that involves **circumscribing spheres of radius R around each point** in a realization of the point process. Thus, $E_V(R)$ is the **expected** fraction of space not covered by these circumscribing spheres. Differentiating (1) with respect to R gives

$$H_V(R) = -\frac{\partial E_V}{\partial R}.$$

- Moments of the nearest-neighbor function $H_V(R)$ arise in rigorous bounds for transport properties of random media. The nth moment of $H_V(R)$ is defined as

$$\langle R^n \rangle = \int_0^\infty R^n H_V(R)\,dR = n\int_0^\infty R^{n-1} E_V(R)\,dR.$$

Series Representations

- For example, for an ensemble,

$$E_V(R) = 1 + \sum_{k=1}^{\infty} (-1)^k \frac{\rho^k}{k!} \int_{\mathbb{R}^d} g_k(\mathbf{r}_1, \ldots, \mathbf{r}_k) \prod_{j=1}^{k} \Theta(R - |\mathbf{x} - \mathbf{r}_j|) d\mathbf{r}_j,$$

where $\Theta(x)$ is the Heaviside step function.

- This series can be rewritten in terms of intersection volumes of spheres:

$$E_V(R) = 1 + \sum_{k=1}^{\infty} (-1)^k \frac{\rho^k}{k!} \int_{\mathbb{R}^d} g_k(\mathbf{r}_1, \ldots, \mathbf{r}_k)\, v_k^{\text{int}}(\mathbf{r}_1, \ldots, \mathbf{r}_k; R)\, d\mathbf{r}_1 \cdots d\mathbf{r}_k,$$

where

$$v_n^{\text{int}}(\mathbf{r}_1, \ldots, \mathbf{r}_n; R) = \int d\mathbf{x} \prod_{j=1}^{n} \Theta(R - |\mathbf{x} - \mathbf{r}_j|)$$

is the intersection volume of n equal spheres of radius R centered at positions $\mathbf{r}_1, \ldots, \mathbf{r}_n$.

- Successive upper and lower bounds:

$$\begin{aligned} E_V(R) &\leq 1 \\ E_V(R) &\geq 1 - \rho v_1(R) \\ E_V(R) &\leq 1 - \rho v_1(R) + \frac{\rho^2}{2} s_1(1) \int_0^{2R} x^{d-1} v_2^{\text{int}}(x; R) g_2(x) dx, \end{aligned}$$

- For a single realization of N points within a large volume V in $\mathbb{R}^d$, we have

$$E_V(R) = 1 - \frac{1}{V} \sum_{i=1}^{N} v_1(R) + \frac{1}{V} \sum_{i<j} v_2^{\text{int}}(r_{ij}; R) - \frac{1}{V} \sum_{i<j<k} v_3^{\text{int}}(r_{ij}, r_{ik}, r_{jk}; R) - \cdots$$

Thus, except for the trivial constant of unity (the first term), $E_V(R)$ can be regarded to be a many-body potential of the general form mentioned earlier.

Reformulations of the Covering and Quantizer Problems

- The covering problem asks for the point process in $\mathbb{R}^d$ at unit density ($\rho = 1$) that minimizes the support of the radial function $E_V(R)$.
- We define $\mathcal{R}_c^{min}$ the smallest possible value of the covering radius $\mathcal{R}_c$ among all point processes for which $E_V(R) = 0$, which we call the minimal covering radius. This is indeed a special ground state in which the "energy" is identically zero (i.e., $E_V(\mathcal{R}_c^{min}) = 0$). Depending on the space dimension d, this special ground state will involve up to n-body interactions, i.e., will truncate at some particular level, provided that $E_V(R)$ for the point process has compact support.
- The minimal covering radius $\mathcal{R}_c^{min}$ increases with the space dimension d and, generally speaking, the highest-order n-body interaction required to fully characterize the associated $E_V(R)$ increases with d.
- Note that for a particular point process, twice the covering radius $2\mathcal{R}_c$ can be viewed as the "effective interaction range" between any pair of points, since the intersection volume $v_2^{\text{int}}(r_{ij}; R)$ is exactly zero for any pair separation $r_{ij} > 2\mathcal{R}_c$.
- Because $v_2^{\text{int}} \geq v_n^{\text{int}}$ for $n \geq 3$, the effective interaction range between any n points for $n \geq 3$ is still given by $2\mathcal{R}_c$.
- The quantizer problem asks for the point process in $\mathbb{R}^d$ at unit density that minimizes the scaled average squared error $\mathcal{G}$ defined as
$$\mathcal{G} = \frac{1}{d}\langle R^2 \rangle = \frac{1}{d}\int_0^\infty R^2 H_V(R)dR = \frac{2}{d}\int_0^\infty R E_V(R)dR.$$
We will call the minimal error $\mathcal{G}_{min}$. Thus, we seek the ground state of the many-body interactions that are involved upon substitution of the series for $E_V(R)$ into the expression above.

Covering and Quantizer Calculations Using $E_V(R)$

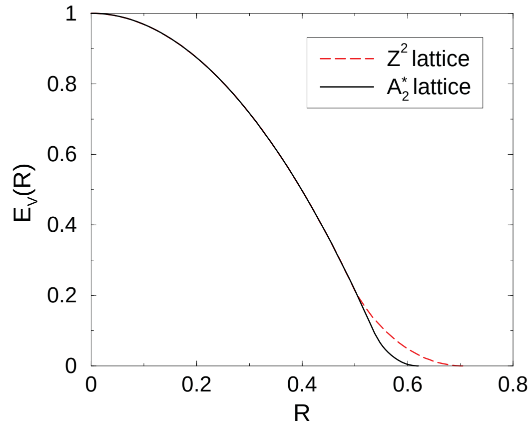


Figure 5: **The void exclusion probability $E_V(R)$ for the $\mathbb{Z}^2$ (square) and $A_2 \equiv A_2^*$ (triangular) lattice have support up to the covering radii $\mathcal{R}_c = \sqrt{2}/2 = 0.7071\ldots$ and $\mathcal{R}_c = \sqrt{2}/3^{3/4} = 0.6204\ldots$, respectively, at unit number density ($\rho = 1$).**

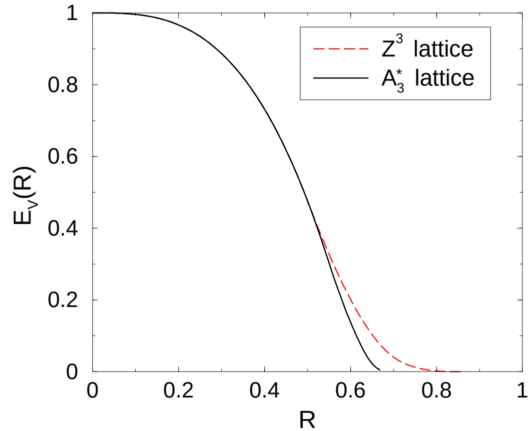


Figure 6: **The void exclusion probability $E_V(R)$ for the $\mathbb{Z}^3$ (simple cubic) lattice and A_3^* (bcc) lattice have support up to the covering radii $\mathcal{R}_c = \sqrt{3}/2 = 0.8660\ldots$ and $\mathcal{R}_c = \sqrt{5}/2^{5/3} = 0.7043\ldots$, respectively, at unit number density ($\rho = 1$).**

Covering Densities for Saturated Packings

- Saturated sphere packings in $\mathbb{R}^d$ should provide relatively thin coverings.
- Why? Surrounding every sphere of diameter D in any saturated packing of congruent spheres in $\mathbb{R}^d$ at packing density ϕ_s by spheres of radius D provides a covering of $\mathbb{R}^d$, and thus the associated covering density θ_s is given by

(1) $$\theta_s = \rho_s v_1(D) = 2^d \phi_s,$$

where ρ_s and $\phi_s = \rho_s v_1(D/2)$ are the number density and packing density, respectively, of the saturated packing.

- **Lemma 1:** *There exist saturated sphere packings in $\mathbb{R}^d$ with density ϕ_s that is bounded from above according to*

$$\phi_s \le \frac{d\ln(d)}{2^d} + \frac{d\ln(\ln(d))}{2^d} + \frac{5d}{2^d}.$$

- Torquato, Uche and Stillinger (2006) found that for RSA saturated packings,

$$\phi_s = \frac{c_1}{2^d} + \frac{c_2 d}{2^d},$$

- Lemma 1 suggests that the fit function for ϕ_s should also include a $d\ln(d)$ correction for large d:

$$\phi_s = \frac{a_1}{2^d} + \frac{a_2 d}{2^d} + \frac{a_3 d\ln(d)}{2^d},$$

Table 6: Covering density θ_s for RSA packings at the saturation state in selected dimensions.

Dimension, d	Covering Density, θ_s	Packing Density, ϕ_s
1	1.4952	0.74759
2	2.1880	0.54700
3	3.0622	0.38278
4	4.0726	0.25454
5	5.1526	0.16102
6	6.0121	0.09394
7	7.0512	0.05508
8	8.0526	0.03145
9	10.0706	0.01769
10	11.0860	0.009834
12	12.1052	0.002955
16	16.2141	2.4740×10^{-4}
17	17.2482	1.3159×10^{-4}
18	18.2848	6.9751^{-5}
24	24.5489	1.4632×10^{-6}

- Saturated RSA packings presumably represent the first non-lattices that yield thinner coverings than the best known lattice coverings beginning in dimension 17.

Bounds on the Quantizer Error

- **Revisiting Zador's Bounds (1982):**

$$\frac{1}{(d+2)\pi}\Gamma(1+d/2)^{2/d} \le \mathcal{G}_{min} \le \frac{1}{d\pi}\Gamma(1+d/2)^{2/d}\Gamma(1+2/d).$$

- **In the large-d limit, Zador's upper and lower bounds become identical:**

$$\mathcal{G}_{min} \to \frac{1}{2\pi e} = 0.058550\ldots \quad \text{as} \quad d \to \infty.$$

- **Consider packings for which the following upper bound on $E_V(R)$ for $R \ge D/2$ is satisfied:**

$$E_V(R) \le (1-\phi)\exp\left\{-\frac{2^d\phi}{1-\phi}\left[\left(\frac{R}{D}\right)^d - \frac{1}{2^d}\right]\right\} \qquad \text{for all} \quad R \ge D/2.$$

- **This leads to an improved upper bound on the quantizer error:**

$$\mathcal{G}_{min} \le \frac{4[\phi\Gamma(1+d/2)]^{2/d}}{d\pi}\left[\frac{(d+2(1-\phi))}{4(2+d)} + \frac{(1-\phi)}{2d}\left(\frac{1-\phi}{\phi}\right)^{2/d}\exp\left(\frac{\phi}{1-\phi}\right)\Gamma\left(\frac{2}{d},\frac{\phi}{1-\phi}\right.\right.$$

Table 7: Comparison of the best known quantizers in selected dimensions to the conjectured lower bound due to Conway and Sloane and the improved upper bound.

d	Quantizer	Scaled Error, $\mathcal{G}$	Conjectured Lower bound	Improved Upper Bound
1	$A_1^* \equiv \mathbb{Z}$	0.083333	0.083333	0.083333
2	$A_2^* \equiv A_2$	0.080188	0.080188	0.080267
3	$A_3^* \equiv D_3^*$	0.078543	0.077875	0.079724
4	$D_4^* \equiv D_4$	0.076603	0.07609	0.078823
5	D_5^*	0.075625	0.07465	0.078731
6	E_6^*	0.074244	0.07347	0.077779
7	E_7^*	0.073116	0.07248	0.076858
8	$E_8^* \equiv E_8$	0.071682	0.07163	0.075654
9	L_9^{AE}	0.071626	0.070902	0.075552
10	D_{10}^+	0.070814	0.070405	0.074856
12	$K_{12}^* \equiv K_{12}$	0.070100	0.06918	0.073185
16	$\Lambda_{16}^* \equiv \Lambda_{16}$	0.068299	0.06759	0.070399
24	$\Lambda_{24}^* \equiv \Lambda_{24}$	0.065771	0.06561	0.067209

RSA Quantizers

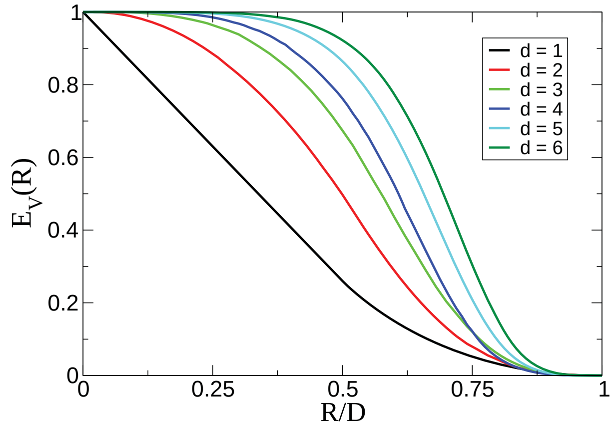


Figure 7: The void exclusion probability $E_V(R)$ for saturated RSA packings of congruent spheres of diameter D for the first six space dimensions.

Table 8: The quantizer errors for saturated RSA packings in the first six space dimensions.

Dimension, d	Quantizer Error, $\mathcal{G}_s$
1	0.11558
2	0.09900
3	0.09232
4	0.08410
5	0.07960
6	0.07799

- RSA saturated sphere packings yield relatively good quantizers as d increases.

CONCLUSIONS

- Covering and quantizer problems have been reformulated as the determination of the ground states of interacting particles in $\mathbb{R}^d$ that generally involve single-body, two-body, three-body, and higher-body interactions.
- These reformulations, which again exemplifies the deep interplay between geometry and physics, allow one now to employ optimization techniques to analyze and solve these ground-state problems.
- This sheds new light on the relationships between the packing, number variance, covering and quantizer problems.
- Quantizer problem is the simplest of the four problems in high-d limit.
- Disordered saturated sphere packings provide relatively thin coverings and may yield thinner coverings than the best known lattice coverings for sufficiently large d.
- Improved upper bounds on the quantizer error have been derived using sphere-packing solutions.
- Disordered saturated sphere packings yield relatively good quantizers.
- Results could have applications to the detection of gravitational waves.

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