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Extreme lattices: symmetries and decorrelation

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Abstract. We study statistical and structural properties of extreme lattices, which are the local minima in the density landscape of lattice sphere packings in d-dimensional Euclidean space $\mathbb{R}^d$. Specifically, we ascertain statistics of the densities and kissing numbers as well as the numbers of distinct symmetries of the packings for dimensions 8 through 13 using the stochastic Voronoi algorithm. The extreme lattices in a fixed dimension of space d ($d \geqslant 8$) are dominated by typical lattices that have similar packing properties, such as packing densities and kissing numbers, while the best and the worst packers are in the long tails of the distribution of the extreme lattices. We also study the validity of the recently proposed *decorrelation principle*, which has important implications for sphere packings in general. The degree to which extreme-lattice packings decorrelate as well as how decorrelation is related to the packing density and symmetry of the lattices as the space dimension increases is also investigated.

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We find that the extreme lattices decorrelate with increasing dimension, while the least symmetric lattices decorrelate faster.

Keywords: Energy landscapes, Structural correlations, Spin glasses, Random/ordered microstructures

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1. Introduction

The sphere packing problem, i.e. finding the densest arrangement of spheres in the Euclidean space of a given dimension d, is a classic problem. Its relevance stems from its applications in mathematics [1, 2] (e.g. geometry and number theory), physics [3–6] (ground states of particles with hard core), communication theory [7, 8] (communication over noisy channels) and combinatorial optimization [9–12]. Though it is very

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simple to formulate, finding an exact solution for the d-dimensional Euclidean space $\mathbb{R}^d$ with arbitrary d has proven to be an extremely difficult task. The packing problem is an optimization problem, and as often happens for these problems, our intuition about the form of the solution (the structure of optimal packings) fails in high dimensions. So far, the answers are only known for $d = 2$ [13], $d = 3$ [14][10], $d = 8$ [15, 16] and $d = 24$ [15, 17], which are '*special*' dimensions for the singular algebraic properties of the resulting optimal lattices.

The simpler version of the problem restricts the set of the packings in which to find the optimum to Bravais lattices, where there is one sphere per fundamental cell. In this paper we will only deal with Bravais lattice (indicated hereafter simply as 'lattices') unless otherwise specified. As the number of dimensions is increased, one expects that the methods of statistical physics should be applicable, even under this restriction, due to the fact that, the number of such configurations grows extremely quickly with d. This situation resembles that encountered in structural and spin glasses. In fact, in principle, the optimization problem admits exact solutions by brute force enumeration of a set of special *perfect* lattices, as it was proven by Voronoi [18] that the densest sphere packing is a perfect lattice (defined in section 2). However, the enumeration procedure becomes impractical (and even intractable) very quickly beyond $d = 8$ where already exactly 10916 lattices are found.

Recently, several approaches have been proposed to discover dense lattice packings from scratch, i.e. without any prior knowledge. All of them exploit the construction due to Voronoi. The sequential linear program of Marcotte and Torquato [19] is a direct reformulation of the Voronoi theory as a convex optimization problem [20]. The Monte-Carlo approach of Kallus [21] also exploits some elements of the Voronoi theory. Both of these methods have proved to be very efficient in discovering the densest lattice packings up to $d = 20$, which turned out all to be the previously known densest lattice packings, but faced problems beyond $d = 20$.

Two of the authors of this paper have recently proposed a stochastic modification of the Voronoi algorithm [22], which allows one to explore the set of perfect lattices (introduced in section 2) in much higher dimensions than the works in [23–25]. This modified algorithm allowed one to study perfect lattices in up to $d = 19$ and rediscover all of the densest known lattice packings although, like in all other numerical approaches [19, 21], the algorithm becomes less efficient as $d = 20$ is approached. The aim of [22] was to explore the set of perfect lattices and reveal the statistical properties of these packings as the dimensionality grew and so a large number of perfect lattices was generated in any dimension from $d = 8$ to $d = 19$ (from various millions in $d = 10$ to hundreds of thousands in $d = 19$). We used the extreme lattices generated by these runs in the present work.

As pointed out above, results applying to any (or sufficiently high) dimension are rather few, mainly in the form of bounds on the maximal packing density. For example, the lower bound due to Minkowski [26], introduced over a hundred years ago, has only been improved linearly in d so far [27, 28]. The *decorrelation principle* introduced recently [29] is a general statement about packings and has important consequences for the packing problem. So an important activity related to the search for the densest

[10] It took over 300 hundred years to prove the solution for $d = 3$.

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packings is the determination of its validity. This principle states that unconstrained correlations (except the one-particle and pair correlation functions, g_1 and g_2) must vanish as $d \to \infty$. In this way the n-body correlation function g_n for any $n \geqslant 3$ can, in the limit, be inferred entirely from a knowledge of the number density ρ and g_2. If this principle is realized, then an exponential improvement on the Minkowski density lower bound for lattices [26] is achieved [29, 30], and the intuition is that the densest packings might be disordered in sufficiently high dimensions. So far there is no generic proof of the decorrelation principle for general optimal sphere packings in high dimensions. However, it has been shown to be true for some specific sphere packings and point processes, including 'ghost' random sequential addition (RSA) packings [31, 32], determinantal point processes [33], equilibrium hard spheres [34, 35], maximally random jammed packings [36, 37], and Gaussian core model [38, 39]. Recent rigorous results on the ground states of the Gaussian-core model in the limit in which it degenerates into hard spheres [40] lend further support to the improved lower bound on the maximal density mentioned above [29, 30] and the decorrelation principle that this bound is based upon.

Therefore an important question is whether any signs of decorrelation can be seen in lattice packings in relatively low dimensions (say, up to $d = 20$, where parctical algorithms exist to generate dense packings) and, if so, how this phenomenon might be linked to the density and symmetry of the packing. In an initial study in this direction, Zachary and Torquato [41] extended the decorrelation principle for ordered packings and showed that decorrelation is clearly visible in several different d-dimensional lattices as well as d-dimensional generalizations of the periodic diamond and kagomé crystals (lattices with a basis) across the first 20 dimensions. However, testing the conjecture for many different lattices and the issue of how decorrelation is related to the density and symmetries of the ordered structures was not examined there.

In the present paper, we will investigate the validity of the decorrelation principle for a special class of lattices, called *extreme* lattices (defined qualitatively below), and examine its relationship to the corresponding lattice packing densities and symmetries. Due to the intrinsic computational difficulties of generating lattices in high dimensions (see figure 1), our study is limited to the examination of extreme lattices in relatively low dimensions $d < 14$, but since we now have the capability of finding many of them in these dimensions [19, 21, 22], we will see that interesting results already emerge. The importance of extreme lattices (a subset of perfect lattices) for the statistical physics aspects of the sphere packing problem follows from the fact that they are the local maxima of the packing fraction, i.e. states whose packing fraction cannot be improved by *any local deformation* of a lattice and therefore have the *strict jamming* property [6, 19]. It is noteworthy that the structure, number and correlations of local density maxima is an important topic in the study of disordered systems [5, 6, 42, 43]. Although lattices are inutitively far from being disordered arrays of spheres, we show that we can learn a lot by applying the same methods used in the context of disordered systems.

Some of the fundamental questions that this research program will shed light on include the following: (i) What are statistical properties of extreme lattices? (ii) Do the densities of typical extreme lattices improve on Minkowksi's lower bound? (iii)

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Are strongly decorrelated packings denser than less decorrelated ones? (iv) Are there special dimensions where decorrelation is weaker/stronger than in neighboring dimensions? (v) Is there a critical dimension in which the best packer becomes as decorrelated as the *typical* extreme lattice? (vi) Is there a critical dimension in which the worst packer becomes *as decorrelated as the typical* extreme lattice? (vii) Does the problem of generating extreme lattices due to the complexity of the density landscape (figure 1) in sufficiently high dimensions share features that arise in the energy landscape of structural glasses?

In order to answer these questions, we have formulated here new descriptors in order to quantify decorrelation and symmetry of lattices. In particular, we introduce a probability measure that enables us to extract a correlation lengthscale to quantify decorrelation. We propose a symmetry index that supposes that the symmetry of a lattice is equal to number of its automorphims. Finally, we devise a metric that quantifies the 'distance' between lattices.

Our major achievements are summarized as follows:

- The set of extreme lattices in some fixed dimension is Gaussian distributed about some mean packing fraction, i.e. there are typical extreme lattices;
- Typical extreme lattices decorrelate faster than the densest lattice or the least dense lattice in a fixed dimension;
- Extreme lattices decorrelate as d increases; the decorrelation is visible already in low dimensions, $d \approx 8$–13;
- In general, more symmetric lattices are less decorrelated; however there are exceptional dimensions where this is not true;
- The worst extreme lattice packing (in terms of packing fraction) is the A_d lattice, defined below[11], is less decorrelated than the best packer in any dimension in the range $9 \leqslant d \leqslant 13$.
- We show that lattices with equal densities in fixed dimension are close to one another in the space of lattices (in terms of the above mentioned 'distance').

The layout of the paper is as follows: we introduce the main definitions that we use later in section 2 and discuss the procedure to discover extreme lattices in section 3. In section 4, we study the statistical properties of the extreme lattices, such as distributions of packing fractions and their moments as well as mean kissing numbers. Section 5 is devoted to the study of symmetries of extreme lattices and their relation to other statistical properties of extreme lattices. In section 6, we focus on the decorrelation properties of the lattices and their connection to statistics of packing fractions and kissing numbers as well as lattice symmetries. Finally, we explore the connection between the geometrical similarity and close densities in the space of lattices in section 7. Our conclusions are presented in section 8.

[11] A_d is a family of lattices, with one member in any dimension d. In 2 and 3 dimensions, they are respectively the triangular and FCC lattices, which are the densest packings in these dimensions.

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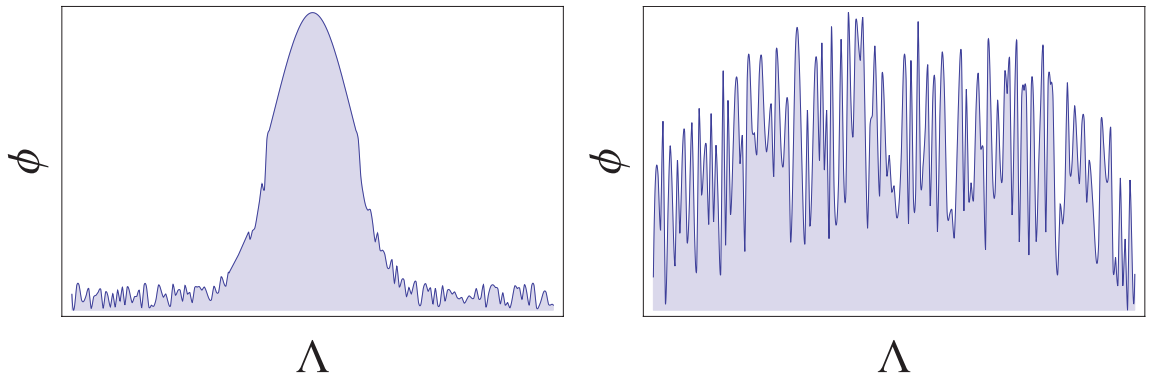


Figure 1. Schematic plot of the density landscape $\phi(\Lambda)$ as a function of lattice Λ for low (left) and high (right) dimensions [43]. For convenience, multidimensional space of lattices Λ is reduced to a one-dimensional line. In low dimensions, the density landscape is relatively simple, reflected by the fact that the densest lattice has a huge basin of attraction and is easily identified. In high dimensions, the density landscape is considerably more complex, reflected by the fact that the basin of the densest lattices becomes comparable to that of other extreme lattices. Thus, the search for the densest lattice in high dimensions becomes increasingly harder as d increases.

2. Definitions

Here we introduce the definitions that we use throughout the paper. A lattice Λ in d-dimensional Euclidean space is defined by its generator matrix A or its Gram matrix $Q = A^t A$ [1]. A lattice admits many equivalent representations in terms of the generator matrix A or the Gram matrix Q: one can rotate the lattice or replace its basis vectors, i.e. the columns of A, with their independent linear combinations. This equivalence is captured by notion of *isometry*: two lattices Q and Q' are called *arithmetically equivalent* if there exists a matrix $U \in \mathrm{SL}_d(\mathbb{Z})$ such that:

$$Q' = U^t\, Q\, U. \tag{1}$$

For example the hexagonal lattice Q_{hex}:

$$Q_{\mathrm{hex}} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \tag{2}$$

has an equivalent representation

$$Q'_{\mathrm{hex}} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \tag{3}$$

which is arithmetically equivalent to Q_{hex} with matrix

$$U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4}$$

A practical way of checking if a given pair of forms is equivalent was developed in [44]: one uses backtrack search to construct an equivalence matrix (if this exists).

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The length of a latice vector represented by a set of integer numbers $\mathbf{v} \in \mathbb{Z}^d$ is given by:

$$\ell(\mathbf{v}) = (\mathbf{v}, Q\mathbf{v})^{1/2}. \tag{5}$$

Lattices have vectors of all lengths, ranging from a minimum value to infinity, and an important object is the set of the shortest vectors of the lattice:

$$\mathrm{Min}(Q) = \{\mathbf{v} \in \mathbb{Z}^d : (\mathbf{v}, Q\mathbf{v}) = \min_{u \in \mathbb{Z}^d \setminus 0^d} (\mathbf{u}, Q\mathbf{u})\}. \tag{6}$$

The number of such vectors is the so-called *kissing number* and is usually denoted by Z as it is the number of spheres in contact with the central sphere, if we set the radius of the sphere to half the length of the shortest vectors $\ell(\mathbf{v})$. Figure 2 shows the shortest vectors of the hexagonal/triangular lattice. The scalar $\lambda(Q) = \ell^2(\mathbf{v}) = (\mathbf{v}, Q\mathbf{v})$ for $\mathbf{v} \in \mathrm{Min}(Q)$ is called *arithmetical minimum* of the lattice and it is also related to the packing properties of the lattice: spheres of radius $\sqrt{\lambda}/2$ placed at the vertices of the lattice give the densest possible packing for this lattice. When talking about a lattice packing we will always imply the packing with the sphere radius $\sqrt{\lambda}/2$.

The *packing fraction* ϕ is the ratio of the volume of the d-dimensional sphere of radius $\sqrt{\lambda}/2$ to the volume of the unit cell of the lattice, given by the determinant of the basis matrix A:

$$\phi = \frac{2^{-d}(\pi\lambda)^{d/2}}{\Gamma(1 + d/2)\det A}. \tag{7}$$

Since the packing fraction decreases at least exponentially fast with the dimension [1], it is convenient to define the *energy*

$$e = -\frac{1}{d}\ln\phi \tag{8}$$

where lower energies corresponds to the better packers [22].

Note that local/global maxima in the packing fraction ϕ are local/global minima in the energy e. The advantage of the energy e over the packing fraction ϕ is its regular behavior as d grows: Minkowski's lower bound on the maximal packing fraction of lattice packings scales like 2^{-d}, while the energy remains a number of order $O(1)$.

A lattice Λ is called *extreme* iff it is *perfect* and *eutactic*. *Perfect* means that any symmetric $d \times d$ matrix M can be expanded as:

$$M = \sum_{\mathbf{v} \in \mathrm{Min}(Q)} \alpha_v \mathbf{v}^t \mathbf{v}. \tag{9}$$

We refer the reader to the examples worked out in [22, 23] to familiarize with the idea of perfect lattices.

An *eutactic* lattice is one for which its inverse Gram matrix has the following decomposition:

$$Q^{-1} = \sum_{\mathbf{v} \in \mathrm{Min}(Q)} \beta_v \mathbf{v}\mathbf{v}^T \tag{10}$$

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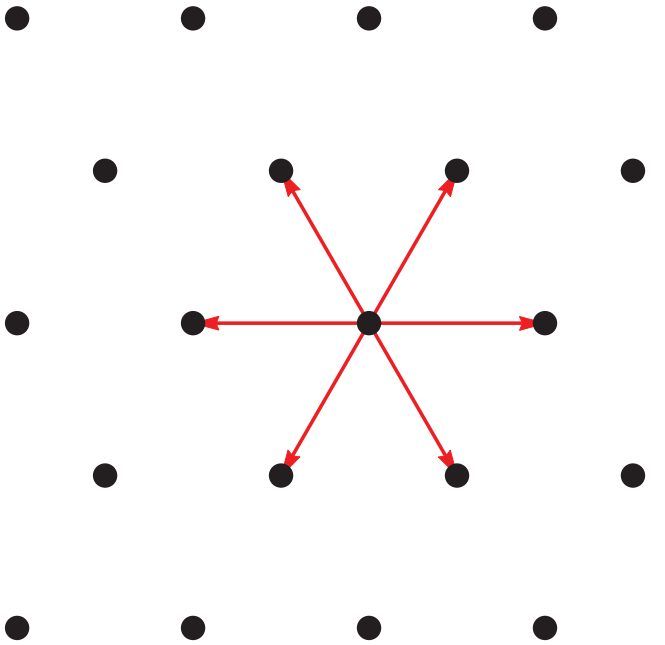


Figure 2. The set of shortest vectors (red) of the hexagonal lattice.

with all positive coefficients $\beta_v > 0$ [23]. As was proven by Voronoi [18], extreme lattices are local maxima of the packing fraction ϕ. As such, they contain important information on the nature of dense packings in high dimensions. In $d = 2$ and 3 there is only one extreme lattice, that realizes the global minimum. However starting from $d = 4$, where there are two extreme lattices A_4, that we define below, and D_4 [1], the number of extreme lattices, i.e. the local maxima of density, grows fast: there are $\sim$2000 lattices in $d = 8$, and many more in higher dimensions.

The central object of the Voronoi theory is the *Ryshkov polyhedron* [45, 46]

$$\mathcal{P}_\lambda = \{ Q \in \mathcal{S}^d_{>0} : \ \lambda(Q) \geqslant \lambda \} \tag{11}$$

where $\mathcal{S}^d_{>0}$ is the set of Gram matrices of all the lattices. The Ryshkov polyhedron is simply a set of all lattices with arithmetical minimum larger than λ. The definition can be rewritten in a more straightforward form:

$$\mathcal{P}_\lambda = \{ Q \in \mathcal{S}^d_{>0} : \ (\mathbf{v}, Q\mathbf{v}) \geqslant \lambda \quad \forall \ \mathbf{v} \in \mathbb{Z}^d \}. \tag{12}$$

From this definitions it is clear, that $\mathcal{P}_\lambda$ is a domain, in the space of lattices, resulting from an intersection of infinite number of planes. One can prove that $\mathcal{P}_\lambda$ is convex and locally is a polyhedron [23] as illustrated in figure 3. This is not trivial since an infinite number of intersecting planes could, in principle, produce an object that is very far from a polyhedron. Figure 3 shows a schematic patch of the Ryshkov polyhedron. An important result due to Voronoi asserts that the maxima of the packing fraction ϕ are attained at the vertices of $\mathcal{P}_\lambda$ [18].

We also use another result due to Voronoi [18, 23]: the set of perfect lattices is finite (up to isometries) and connected. Namely, for any perfect lattice Q one can always compute a special subset of perfect lattices, which are called its *neighbors* [23, 47]. These are the endpoints of the edges of the Ryshkov polyhedron coming out

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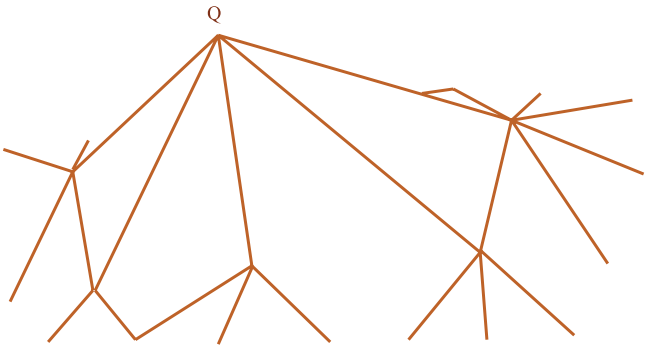


Figure 3. A schematic drawing of a patch of the Ryshkov polyhedron $\mathcal{P}_\lambda$ defined by (12). A perfect lattice defined by its Gram matrix Q is a vertex of the polyhedron $\mathcal{P}_\lambda$. The edges radiating from Q join lattices reachable using Voronoi's algorithm (Voronoi neighbors) and form the Voronoi domain of the lattice.

the vertex Q on figure 3. Repeating this procedure for every neighbor, one can, in principle, generate the complete set of perfect lattices. This turns the set of perfect lattices into a graph. We refer to it as *the Voronoi graph* throughout the paper.

An example of extreme lattice is the A_d family of lattices [1]. The Gram matrix of the lattice in d dimensions reads:

$$Q_{A_d} = \begin{pmatrix} 2 & -1 & 0 & 0 & \cdots \\ -1 & 2 & -1 & 0 & \cdots \\ 0 & -1 & 2 & -1 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{13}$$

Geometrically the A_d lattice is defined a set of all points $\mathbf{x} \in \mathbb{Z}^{d+1}$ with integer coordinates, such that $\sum_i x_i = 0$. The A_2 and A_3 are the hexagonal, or triangular, and FCC lattices in $d = 2$ and $d = 3$ respectively. These are the densest lattices in respective dimensions. However beyond $d = 4$ the A_d are no longer the densest lattices. As space dimension increases, they become *sparse*, i.e. have low density, as we will see below.

3. Generation of sets of extreme lattices

Unlike the case of perfect or eutactic lattices where algorithms exist which do, in principle, enumerate all such lattices [18, 48], no algorithm is known that generates directly extreme lattices in a sequential way (like the Voronoi algorithm does for perfect lattices). One has to start either from perfect lattices and then check them for eutaxy or do the opposite: generate eutactic lattices [48] and check for perfection (the former procedure is algorithmically faster, and it is the one that we use in this paper). It is worth mentioning that a recent algorithm manages to generate random dense and maximally jammed packings [19, 20, 43] therefore achieving extremity without requiring separately perfectness and eutacticity. The term ' *random*' refers to the fact the algorithm starts from a random lattice and compresses it into an extreme one. Therefore this

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algorithm also samples the set of extreme lattices and generates its random representative[12]. As we said, the algorithm for generating perfect lattices and check for their eutacticity is simpler, and we have implemented it in a randomized variant in [22]. The full details of the algorithm are presented in [22], so only an outline is given below. Since A_d lattices are extreme in any dimension, they can be used as a starting point of both the original and stochastic Voronoi algorithms. It is also possible to pick any of the perfect lattices generated by previous runs of the algorithm. The major difference of the stochastic algorithm with the original Voronoi algorithm, is that instead of computing all the neighbors of a perfect lattice Q at every step as was described above, in the stochastic variant of the algorithm one only computes one neighbour at random (however the weighting of the neighbours is not uniform). This generates a random walk on the set of all perfect forms. Computation of all the neighbors becomes computationally prohibitive as d and the kissing number Z increase, as it is equivalent to the notorious polyhedron representation conversion problem [23, 25]. The number of perfect lattices is conjectured [22] to grow superexponentially with dimension and the number of eutactic (not necessarily perfect) lattices grows even faster [48, 49]. We conjecture that the number of extreme lattices is growing at least exponentially fast with the dimension of space. Yet the fraction of perfect lattices that are also eutactic discovered by our stochastic algorithm decreases rapidly with space dimension as illustrated in table 1. The increase of the fraction of lattices in $d = 10$–11 is related to the bias of the algorithm towards the denser lattices and to the fact that the Voronoi graph in these dimensions is relatively small compared to dimensions $d \gtrsim 15$ [22], which makes the random walk biased towards extreme lattices. In higher dimensions the size of the graph quickly negates the bias (not shown).

These observations make generation of representative sets of extreme lattices a challenging task, and this is the main limitation of our work. Another limitation is that the number of extreme lattices discovered in a single run of the randomized Voronoi algorithm tends to be wildly changing from run to run. Specifically, there are two difficulties encountered: first, the fraction of extreme lattices (among the perfect lattices generated) drops sharply above $d = 12$. The drop is caused by a steep inflation of the Voronoi graph, so that non-equivalent extreme lattices have larger and larger separation (in terms of distance on a graph) as the dimension of space is increased beyond $d \approx 14$. In other words, the average number of steps, i.e. lattices that are only perfect, between the discovery of the two consecutive extreme lattices increases rapidly for $d \gtrsim 14$. Second, the appearance of many equivalent copies of the same lattice starts becoming a problem, much more important for extreme lattices than it is for perfect lattices (extreme lattices seem to have more representations than perfect lattices). If we bias the random walk with a Metropolis-like rule by introducing an *effective* temperature and taking the (logarithm of) the packing fraction as configurational energy, we increase the fraction of extreme lattices discovered among the perfect lattices, however, for $d \geqslant 13$ they turn out to be mostly equivalent copies of a small set of extreme lattices.

For $d \leqslant 13$ a successful strategy is to generate sufficiently long random walks of 10^6–10^7 steps, with a Metropolis bias, and restart the procedure many times. The instance $d = 13$ seems to be a borderline case since a random walk of $6 \cdot 10^6$ steps

[12] Note however that the extreme lattices generated in [19] are mostly equivalent copies of few extreme lattices, mostly, the densest one in the corresponding dimension.

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Table 1. Fraction x of perfect lattices that are also extreme, as a function of dimension. The numbers in $d = 6$, 7, 8 are exact, while the fractions for $d > 8$ are based on the output of the stochastic algorithm [22]. The increase of the fractions in $d = 10$–11 is likely to be related to the bias of the algorithm and is not supported by results in $d \geqslant 13$ (not shown).

d	5	6	7	8	9	10	11	12	13
x	1	0.857	0.909	0.22	0.156	0.35	0.32	0.31	0.17

starting from A_{13} yielded $2 \cdot 10^4$ extreme lattices. An estimate of a similar run in $d = 14$ would give only a few hundred lattices with substantial increase of the running time. For $d \geqslant 14$ the only possibility we are left with is to perform repeated runs at moderate temperatures, extract extreme lattices, check them for equivalence and merge the set all together and perform an equivalence checks over the resulting set. Following this approach, we were able to collect from 200 to a few thousand extreme lattices for $d = 14$–19.

Since, we cannot guarantee that lattices in such sets are representative of the typical properties of the extreme lattices, we focus on the range $d = 8$–13. We discuss the generating procedure and its alternatives in appendix C.

4. Statistics of packing fraction and kissing number

We start by studying statistical properties of extreme lattices. We study the same quantities—energy $e = -\log(\phi)/d$ and kissing number Z—as was done in the case of perfect lattices [22].

The first issue we would like to discuss is whether statistics of energy and kissing number of extreme lattices is different from that for perfect lattices. As explained in [22] the randomized Voronoi algorithm is hardly uniform in the choice of a neighbor of a given perfect lattice. This is due to the large variance in the dimensions of the facets of the Ryshkov polyhedron [22]. In order to render it more uniform we have biased the random walk. This gave a better sampling of the perfect lattices (as measured in terms of less repetitions) and the same is true for the extreme lattices as well.

We notice however little difference between the two algorithms and a net tendency of the extreme lattice distribution towards the densest lattices (see figures 4 and 6. Figure 5, showing the energy PDF for perfect lattices in $d = 8$–19 is presented here for comparison). In brief, extreme lattices are typically denser than perfect lattices (see figure 4).

At this point we notice a curios phenomenon: although in $d = 3$ dimensions the lattice A_d is the best packer, as the number of dimensions increases it becomes *consistently* the least dense among the extreme lattices. This is a known conjecture by Coxeter [50, 51] and we found evidence for it in our numerics.

It is also worth pointing out that the average energy $\langle e \rangle$ of extreme lattices is lower than that of the perfect lattices for the range of dimensions studied. This might have important implications, since we conjectured in [22] that typical perfect lattices improve upon the Minkowski bound.

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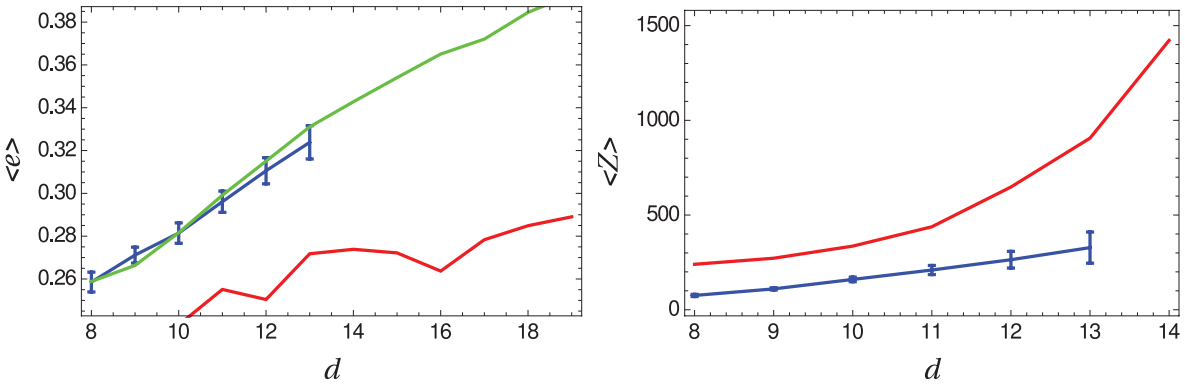


Figure 4. *Left.* Average energy of perfect (green, top curve) and extreme (blue, middle curve) lattices as a function of dimension. The red (bottom) curve is the energy of the best known packings. *Right.* Average kissing number $\langle Z \rangle$ of extreme lattices (blue, bottom curve) as function of dimension. The red (top) curve represents the kissing numbers of the densest known packings. Error bars are variance of the distributions.

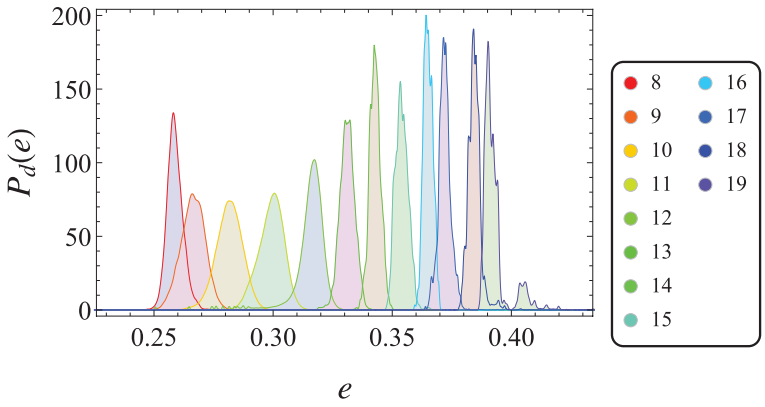


Figure 5. Probability distributions for energy of perfect lattices in $d = 8$–19.

5. Symmetries of extreme lattices

The next problem we address, before proceeding with the decorrelation properties, are the symmetries of the extreme lattices. We need an appropriate measure of how symmetric is a sphere packing corresponding to a given lattice. The symmetries of a lattice Λ, defined by its Gram matrix Q, and associated packing are quantified by an *automorphism group* $\mathrm{Aut}(Q)$:

$$\mathrm{Aut}(Q) = \{ U \in \mathrm{GL}_d(\mathbb{Z}) : U^t \, Q \, U = Q \}. \tag{14}$$

This is the set of linear, integer changes of variables in $\mathbb{Z}^n$ that map the lattice on itself, i.e. the set of all 'rotations' in space, under which the lattice points map onto themselves[13]. This is a simple direct probe for the symmetry of a sphere packing. For example the square lattice in two dimensions has Gram matrix

[13] If $\Lambda = A\mathbb{Z}^d$ and $Q = A^t A$, then every $U \in \mathrm{Aut}(Q)$ defines an orthogonal transformation $O \in SO(d)$ such that $AU = OA$ holds.

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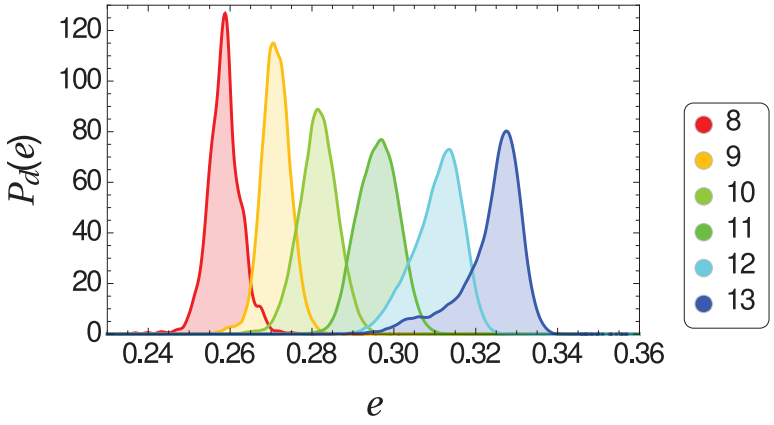


Figure 6. Probability distributions for energy extreme lattices in $d = 8$–13. Color goes from red, $d = 8$ to blue, $d = 13$. Up to $d = 13$ the sampling is good. The behavior of the distributions is similar to that of the distributions for the perfect lattices, shown on figure 5.

$$Q_{\text{sq}} = \mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{15}$$

and therefore the group

$$\text{Aut}(Q_{\text{sq}}) = \{ U \in \text{GL}_2(\mathbb{Z}) : U^t U = \mathbf{I} \}. \tag{16}$$

This is the group of signed permutations, which has 8 elements in 2 dimensions (in general $2^d d!$, for d dimensions).

On the other hand, the hexagonal (or triangular) lattice has Gram matrix

$$Q_{\text{hex}} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \tag{17}$$

has the following automorphism group

$$\text{Aut}(Q_{\text{hex}}) = \left\langle \mathcal{A}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \mathcal{A}_2 = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} \right\rangle \tag{18}$$

of 12 elements, which are generated from the above two generators of the group[14]. Therefore the hexagonal lattice has 50% more symmetries than the square lattice (12 instead of 8) and this corresponds to our intuitive notion of the hexagonal lattice being more symmetric than the square lattice. A crude measure of this is the number of elements in $\text{Aut}(Q)$, which we denote as $|\text{Aut}(Q)|$. Notice as well, that while the definition of the group relies on the Gram matrix Q, which is itself defined up to an isometry V, the $|\text{Aut}(Q)|$ does not depend on V. Notice as well, that while the above $d = 2$ case suggests that the densest lattice is also the most symmetric among the lattices, this is not so in higher dimensions, as we will see.

We adopt as a measure of the symmetry of a lattice the size of it automorphism group $|\text{Aut}(Q)|$. As the size of the group can be exponentially large in d for certain

[14] The reader can verify that the group is indeed closed and has 12 elements. It helps to notice that $\mathcal{A}_{1,2}$ are roots of the identity, in particular $\mathcal{A}_1^2 = 1$ and $\mathcal{A}_2^6 = 1$.

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lattices Q, it is more convenient to work with its logarithm: we define the symmetry exponent s of a lattice Q as:

$$s = \ln|\mathrm{Aut}(Q)|/d. \tag{19}$$

This quantity is of order $O(\ln d)$ even in the case of A_d, which has a fairly large symmetry group in high dimensions[15]. We have used the original code [44] by Plesken and Souvignier to compute the size of the automorphism groups $\mathrm{Aut}(Q)$.

It is also worth pointing out at this stage, that the number of symmetries is the simplest possible measure of how symmetric a packing is. Both the worst and the best packers in the range of dimensions studied have large symmetry groups. However the computing time needed to identify the groups is typically much smaller for the bad packers, like A_d, D_d than for dense lattices. We do not currently have an explanation of this fact, yet it suggests that more subtle measures of symmetries then their number might exist.

5.1. Symmetries

We first look at the distribution and the moments of s for extreme lattices. Figure 7 shows three curves: the mean $\langle s\rangle$ over the ensemble of extreme lattices, the s as a function of dimension for the best (middle curve) and the worst (top curve) packers. In all cases, the worst packer is A_d. We consistently find for $d > 10$ that the best *and worst* packers have high symmetry with $s \simeq 1$ for the best and $s \simeq 2$ for the worst, and there is always an exponential gap between the two. This similarity between the best and the worst can be understood as they are both the result of a global optimization (a maximum and a minimum of the same function). The trend as the number of dimensions increases is that of a *decreasing* of the number of symmetries s in the best packer while the number of symmetries in the *worst* packer A_d increases logarithmically (we have a crossing at $d = 9$). Typical extreme lattices have much less symmetry, $\langle s\rangle \approx 0.1$, which translates into slowly increasing $|\mathrm{Aut}|$ from 2.23 for $d = 8$ to 3.67 for $d = 13$. This tells us that typical extreme lattices have, essentially, no symmetries, especially if compared to the best and worst cases.

To support this statement, we study the distribution of s for $d = 8$–13, which is shown in figure 8. The distributions of s feature the main peak that shifts to smaller values of s as d increases.

5.2. Correlation between packing fraction, kissing number and symmetries

In this section we study the dependence of $|\mathrm{Aut}(Q)|$ on the lattice energy or kissing number. The results are shown in figure 9. We see that typical extreme lattices have low symmetry (small number of symmetries), sometimes as low as just two transformations, while the best/worst packers are highly symmetric. However it is not difficult to find lattices which do pretty well in packing while keeping the number of symmetries low and it is possible to find extremely high kissing numbers in packings which have

[15] As $|\mathrm{Aut}(A_d)| = 2(d+1)!$, strictly speaking $s(d) = \ln d + O(1)$ using Stirling's formula, but for such small d we do not see the logarithmic growth.

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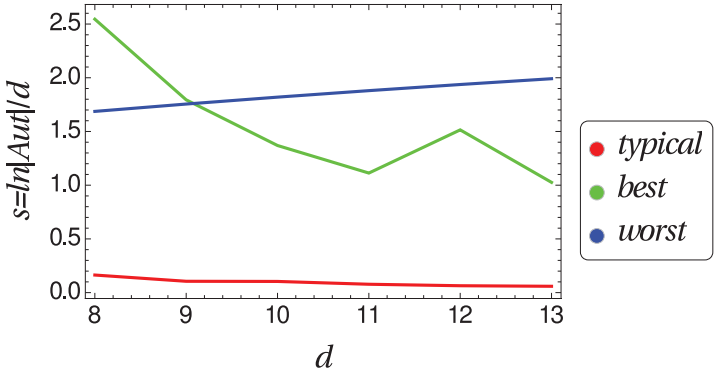


Figure 7. The mean symmetry exponent $s = \ln|\mathrm{Aut}|/d$ of extreme lattices (red, bottom), the best (green, middle curve) and the worst (blue, top curve) packers. The *mean* curve shows smooth behavior, while the extreme cases curves are less regular. In particular the $d = 12$ is special. The least dense case, which we verified being consistently A_d, has higher symmetry than the densest lattices for all dimensions >8 and asymptotically (see appendix B) $\ln|Aut(A_d)|/d \simeq \ln d - 1 + \frac{3}{2}\ln d/d + \ldots$.

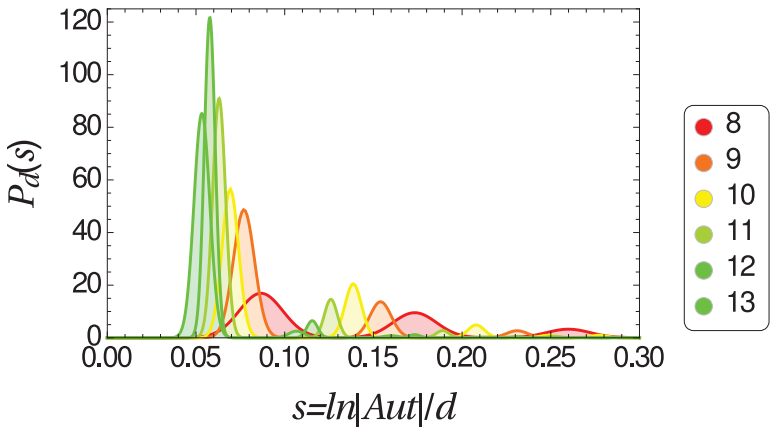


Figure 8. The distributions of the symmetry exponent s of extreme lattices for $d = 8$–13. Color gets colder as dimension d is increasing. The peak of the distribution shifts to smaller values of s with increasing dimension.

s value less than half that of the best kisser. This also becomes more accurate as the dimension is increased.

As the dimension d increases the A_d lattices become more distant from the rest of the lattices with extremely huge symmetry groups. At the same time, they become the worst packers. A similar behavior is observed if $|\mathrm{Aut}(Q)|$ is plotted against the kissing number, as illustrated in figure 10.

6. Decorrelation principle for lattices

In this section, we study the decorrelation properties of extreme lattices and their connection to density and symmetry of a lattice, which is one of the main subjects of this

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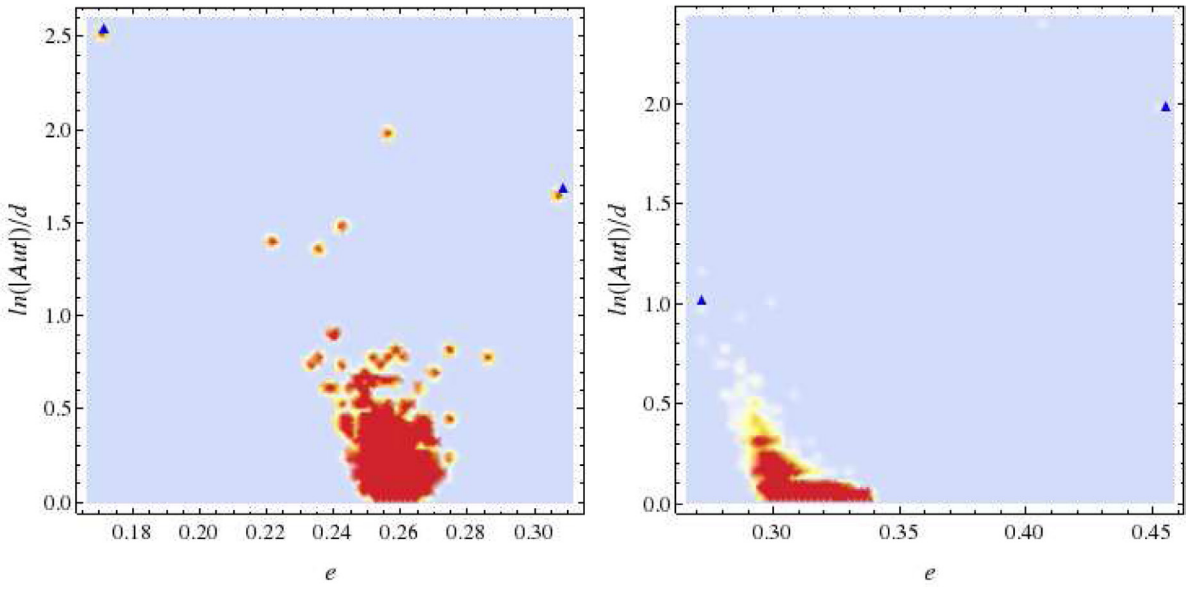


Figure 9. The symmetry exponent s of a lattice as function of energy for $d = 8$ (left) and $d = 13$ (right). As there are thousands of points in the plot, we have resorted to color coding for the frequency of such points, where red is the most frequent and light blue is empty regions. The intermediate dimensions have similar scatter plots. The dark blue triangular marks indicate the best and the worst known packers. One concludes that the densest and the sparsest (A_d) lattices have (much) higher number of symmetries than typical extreme lattices.

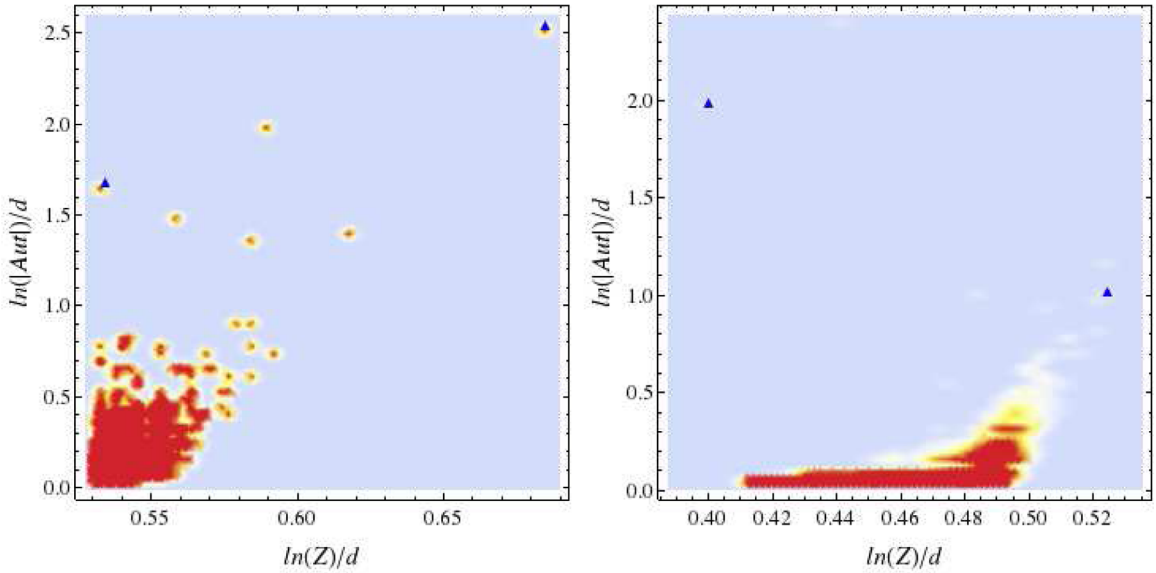


Figure 10. The symmetry exponent s of a lattice as function of the kissing number for $d = 8$ (left) and $d = 13$ (right). As there are thousands of points in the plot, we have resorted to color coding for the frequency of such points, where red is the most frequent and light blue is empty regions. The intermediate dimensions have similar scatter plots. The (blue) triangular marks indicate the best and the worst known kissers. One concludes that the densest and the sparsest (A_d) lattices have (much) higher number of symmetries than typical extreme lattices.

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paper. The *decorrelation principle* [29] states that all correlations except the pair correlations vanish as dimension of space is increased. It has been shown to be rigorously true for some specific sphere packings and point processes [29–31, 33]. Moreover, there is direct theoretical and numerical evidence that decorrelation is already evident in disordered systems in low dimensions (up to 20 dimensions) as d increases [32, 34–39, 52]. It is therefore of interest to study if it holds for extreme lattices in relatively low dimensions and then to examine its consequences.

In particular, we want to study how the decorrelation properties of extreme lattices, i.e. the local maxima of the packing fraction, changes with dimension and how they depend on energy/kissing number of a lattice for a fixed dimension. The latter case requires a method to compare decorrelation properties of different lattices. First, we rescale all extreme lattices to have unit length shortest vectors, i.e. we set the arithmetical minimum $\lambda = 1$. We use this convention throughout the rest of the paper. This way different lattices (in a given dimension) correspond to different local arrangements of hard spheres around a central sphere. The extreme lattices, as we said, give the packings whose density cannot be improved by any infinitesimal deformation of a lattice.

A direct test of the decorrelation properties of a lattice, would be to check whether higher-order correlators, like the three-body correlator g_3, factorize into products of density ρ and pair correlators g_2. This is computationally difficult and we set it aside for future work. A second, less direct, test of the validity of the conjecture explores the implication of the decorrelation principle, that the pair correlator g_2 contains less and less features and approaches 1 for all distances as the dimension d is increased. This second possibility is feasible, instead, since the pair correlations are easier objects to compute numerically and only requires quantitative measure of features of g_2. More precisely, we study whether g_2 reveals decorrelation and how this is related to dimension/energy/kissing number as the number of dimensions is increased.

The pair correlation function $g_2(r)$ is defined as a probability of finding a particle at distance r given there is a particle at the origin. The g_2 is also equal to derivative with respect to R of the number of particles inside a sphere of radius r. For Bravais lattices $g_2(r)$ is a set of δ-functions:

$$g_2(r) = \sum_{k>0} g_k \delta(r - r_k)$$
$$g_k = \frac{Z_k}{d 2^d \, r_k^{d-1} \phi} \tag{20}$$

where ϕ is the packing fraction, Z_k is the number of lattice points in the kth shell and r_k is the length of the lattice vectors in the shell. We refer to the series (20) as *g_2-series* in the remainder of the paper. For all the lattices, considered in our paper[16], their complete $g_2(r)$ series can be computed exactly through the knowledge of a finite piece of their theta series [1, 53]:

$$\theta_\Lambda(q) = \sum_{\mathbf{v}\in\Lambda} q^{\mathbf{v}^2}. \tag{21}$$

[16] This statement holds for any lattice with rational Gram matrix, i.e. for any perfect/extreme lattice.

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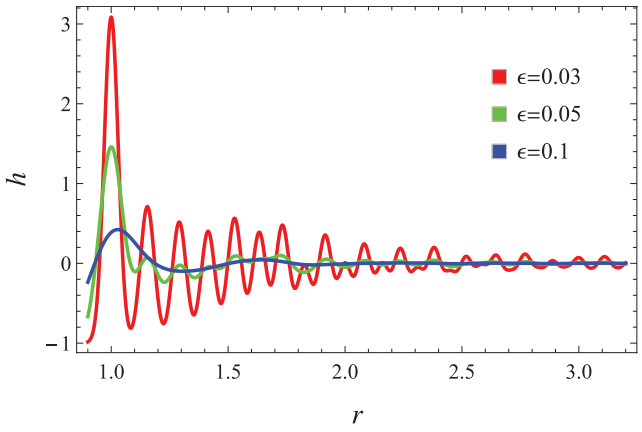


Figure 11. The smoothed h functions for a typical $d = 8$ extreme lattice as defined in (23) with $\epsilon = 0.03, 0.05, 0.1$. The δ-functions are smoothed into Gaussians. The correlator goes to 0 for large distances.

However the size of the required piece of the theta series can be substantial and the algorithm, relying heavily on the theory of modular forms, is non-trivial. The pair function g_2 has been computed by this method only for certain lattices. When this was not possible, we have resorted to a numerical method, which consists in counting all points in the lattice within a spherical region of changing radius, up to a maximum distance of few shortest vectors lengths, depending on the dimension of space. The higher space dimension, the smaller the maximum distance we have used due to computational costs.

The original decorrelation principle was developed for disordered systems. Its application to lattices requires different descriptors to detect it. One challenge is the obvious long-range order present that makes g_2 a sum of δ-functions, which is strictly speaking not one anywhere. However, recently Zachary and Torquato [41] showed, that the decorrelation can be extended to the case of periodic systems, including lattice packings, if one studies the *smoothed* pair correlators:

$$g_2(r;\epsilon) = \frac{1}{\epsilon\sqrt{2\pi}} \sum_{k>0} g_k \exp\left[-\frac{(r-r_k)^2}{2\epsilon^2}\right] \tag{22}$$

$$h(r;\epsilon) = g_2(r;\epsilon) - 1 = -1 + \frac{1}{\epsilon\sqrt{2\pi}} \sum_{k>0} g_k \exp\left[-\frac{(r-r_k)^2}{2\epsilon^2}\right] \tag{23}$$

where the δ-functions are replaced by suitably chosen approximations (the Gaussians in the above equations), which converge to a δ-function for small values of ϵ. The smoothed g_2 should go to 1 uniformly as $d \to \infty$ and fixed ϵ, as the delta functions become denser for large r. An example of the smoothed g_2 correlator for a typical extreme lattice in $d = 8$ is presented in figure 11. The effect of decorrelation is then to suppress any oscillations from 1. In terms of h, we expect that

$$h(r) \to 0 \quad d \to \infty, \tag{24}$$

for any $r > 1$ (recall that we have normalized all the lattices to have unit-length shortest vectors.) and a fixed ϵ. The order of the limits $d \to \infty$ and $\epsilon \to 0$ is important in this

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case: taking $\epsilon \to 0$ before $d \to \infty$ always results in δ-like pair correlator. In what follows we use $\epsilon = 0.1$ unless otherwise stated.

Having found the tools needed to extend the decorrelation principle to lattices, we can either study how specific d-dimensional lattice decorrelates with d [41] or look at decorrelation properties of lattices for a fixed d. For the latter, we need to define a quantitative measure of the decorrelation of a lattice, so that comparison of different lattices is possible. To do that, we have exploited the observation that the smoothed lattice g_2, loses the structure and approaches 1 on shorter and shorter distances as d is increased [41]. If one wants to define a *correlation length* ξ over which the smoothed g_2 looses its structure, one is faced with various choices. One possibility is to set $\xi = \langle r \rangle$ where the average is taken with the appropriately normalized $h^2(r)$ as a probability measure (the choice of h^2 is dictated by convenience; one can use any other positive function of h). Another possibility is to use the cumulative function

$$\chi(r, \epsilon) = \frac{1}{\int_1^\infty \mathrm{d}r\, h^2(r, \epsilon)} \int_1^r \mathrm{d}r\, h^2(r, \epsilon). \tag{25}$$

We set ξ so that $\chi(\xi, \epsilon) = \eta$ with $\eta \sim 0.9$–0.99. This last definition is close to the definition of the *order metric* used to quantify disorder in materials [54]. Specifically, it would measure the radius (in shortest vectors) of a sphere containing 90%–99% of the order metric.

Still another possible definition uses the cumulative function $\chi(r, \epsilon)$. One can study its behavior as $r \to \infty$ and extract a characteristic length which determines the approach to the asymptote. We have found that two different correlation lengths can be extracted with this definition from the smoothed lattice two-point correlators, describing the small-r and on the large-r behaviors of the g_2 [55].

Irrespective of the method used ($\langle r \rangle$ or χ) the smaller ξ the more *decorrelated* is the lattice. We will see below that the decorrelation length is well correlated with symmetry (the larger the lattice symmetry group, the larger ξ).

It is worth stating at this point that g_2 does not define lattice uniquely for $d > 3$. The g_2 series and the related θ-series can be the same for different lattices, except in $d = 2$, 3. Counterexamples exist in $d \geqslant 4$, i.e. non-equivalent lattices which have identical g_2-series to all orders [56–60]. The exhaustive study of decorrelation properties of (lattice) packings would require analysis of factorization of higher-order correlators.

6.1. Decorrelation and energy

We first study the correlation between the decorrelation length ξ and the energy e. We have found that the method used to compute the length ξ is quite stable: both the analysis of χ- and of $\langle r \rangle$-methods give qualitatively similar results. Moreover the results of the χ method do not change qualitatively for different thresholds η, if they are taken large enough: $\eta \gtrsim 0.9$. In what follows we present the results obtained using the χ-method with $\eta = 0.95$.

Looking at the scatter plots for $d = 8$,12,13 in figure 12, we see that typical extreme lattices have smaller length ξ. i.e. they are more decorrelated, than the best and the worst packers. In $d = 13$ the densest lattice is as much decorrelated as most extreme lattices as we see in figure 12. The reason for such behavior of the best packer in

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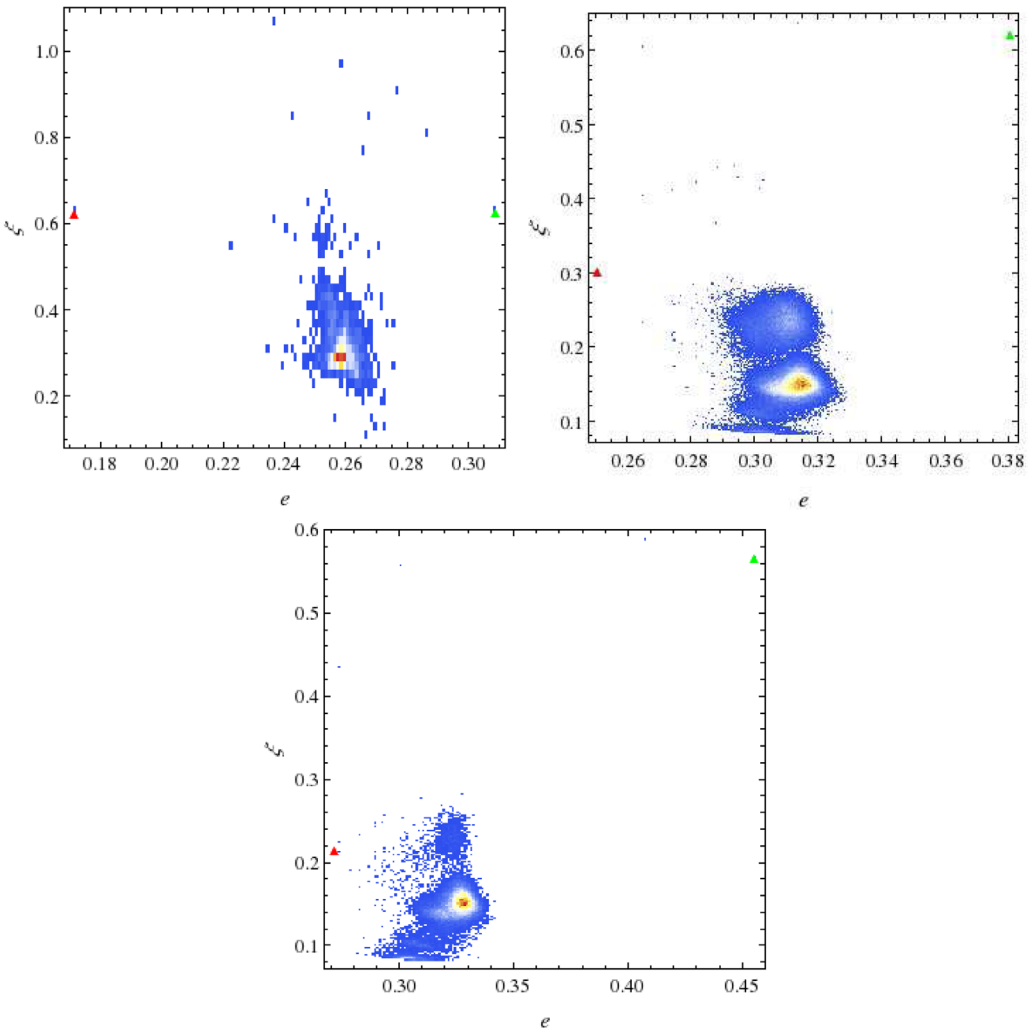


Figure 12. Scatter plot of correlation length ξ versus energy $e = -\log \phi/d$, $d = 8$, 12, 13 (top left, top right and bottom respectively). The smoothing parameter $\epsilon = 0.1$ (see (23)). The red and green triangular marks label the densest and the least dense extreme lattices. Typical extreme lattices have smaller correlation length in comparison with lattices having high or low energy. The relative closeness of the densest lattice to the bulk of typical extreme lattices in $d = 13$, is a peculiarity of $d = 13$, where the densest lattice is more decorrelated than expected, as explained in the text.

$d = 13$ is shown in figure 14, where the smoothed g_2 correlators for the best packers in $d = 12,13,14$ are compared: the g_2 in $d = 13$ has less structure than the smoothed g_2 in the neighboring dimensions. Such decorrelation properties as a function of dimension d were conjectured in [30].

6.2. Decorrelation and symmetries

Next we study the correlation between ξ, that quantifies decorrelation properties, and the size of the symmetry group of a lattice as measured by s. The results are presented in figure 13. We see that ξ and s are correlated (although the correlation is not striking):

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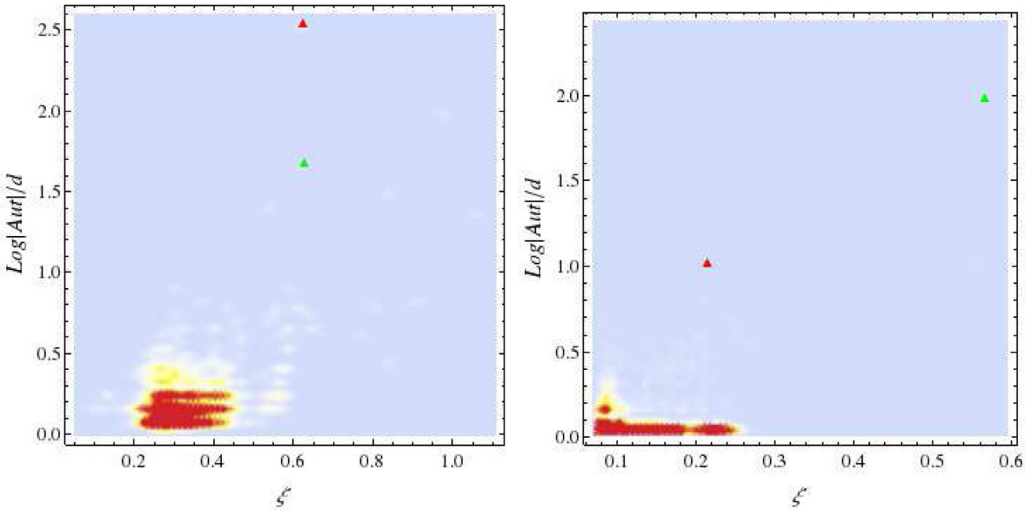


Figure 13. Symmetry exponent s of extreme lattices versus correlation length ξ (computed with the χ method, $\eta = 0.95$), for $d = 8$ (left) and $d = 13$ (right). The smoothing parameter $\epsilon = 0.1$. As there are thousands of points in the plot, we have resorted to color coding for the frequency of such points, where red is the most frequent and light blue is empty regions. The intermediate dimensions have similar scatter plots. One observes a trend for extreme lattices with lower symmetry to have smaller correlation length ξ.

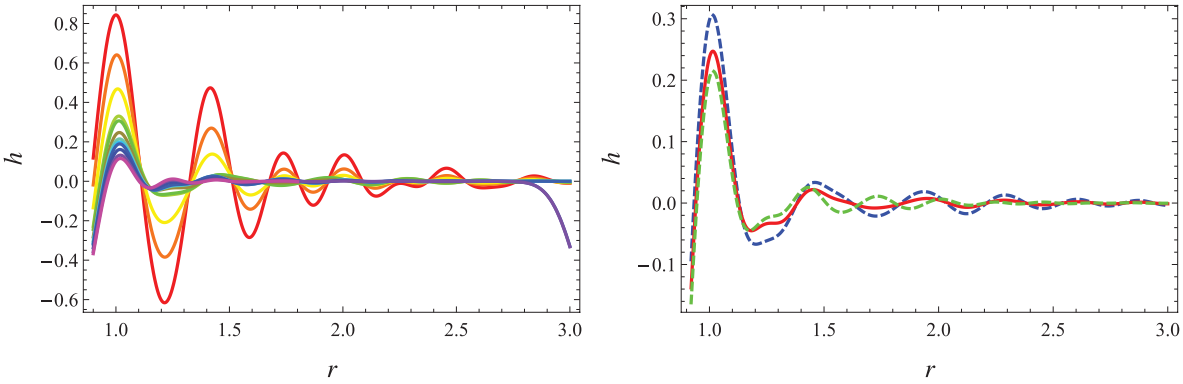


Figure 14. *Left.* The smoothed h correlator (see (23)) with $\epsilon = 0.1$ of the best packers in $d = 8$–19. The color is darker for larger d. *Right.* The same plot restricted to $d = 12$–14. The smoothed g_2 for the best packer in $d = 13$ (red, solid) has less structure than the smoothed g_2 in $d = 12$ (blue, dashed) and $d = 13$ (green, dashed).

lattices with larger symmetry groups typically have also larger correlation lengths ξ, i.e. they are less decorrelated. More precisely, we have found, that the typical extreme lattices, that we have introduced above and that have very low number of symmetries, are the fastest to decorrelate. The least dense lattices, like A_d and D_d, that have huge symmetry groups already in moderately high dimensions ($\mathrm{Aut}(A_{20}) = 102\,181\,884\,343\,418\,880\,000$ and $\mathrm{Aut}(D_{20}) = 2551\,082\,656\,125\,828\,464\,640\,000$) also have large correlation lengths compared to the typical extreme lattices. The case of the (known) densest lattices is special: While most of the time there is the correlation between the number of symmetries and decorrelation, there are special dimensions where the densest lattice is particularly decorrelated, for example in $d = 13$, as illustrated in figure 13.

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As the dimension increases, the difference in correlation between the best packers and typical ones starts to decrease, as one can see in figure 14 which shows the smoothed g_2 correlators for the best packers in $d = 8$–19. It is evident that, while for $d = 8$ the best packer is much less decorrelated than the typical extreme lattice in $d = 8$, for $d = 13$ the difference shrunk and we expect this tendency to be only more evident in higher dimensions.

7. Correlations between lattices and glassiness

We have seen that typical extreme lattices in moderately high dimensions are quite homogeneous as to what concerns packing fraction and symmetries (and we conjectured that this becomes more and more true as the number of dimensions is increased). A series of natural questions arise: what other common features are there of typical extreme lattices? Are best packers so different from the typical ones that we could single them out by using a different metric than the packing fractions? Do they cluster in some appropriate sense, resembling local minima of the free energy of mean-field glasses [61]?

To answer these questions, a good starting point is to analyze whether the lattices that are close in energy are also similar in real space configuration. The latter requires a definition of distance $\rho(\Lambda, \Lambda')$ between lattices Λ, Λ' as a measure of geometric similarity.

Defining a workable metric in lattice space is a non-trivial problem as there might be very different presentations of the same lattice. Since lattice can be represented by many equivalent Gram matrices, the latter cannot be used tout-court to construct the metric (see appendix A for more details) and one has to scan for different presentations of the same lattice.

An alternative possibility is to use theta series associated to a lattice [1]:

$$\theta_\Lambda(q) = \sum_{v \in \Lambda} q^{|v|^2}. \tag{26}$$

It is possible to define a distance in the space of lattices with the help of theta series, however its computation represents a serious mathematical problem (see appendix A for discussion of possible metrics for lattices). One could think of computing the distance between θ's in function space.

The idea is good but computing the θ, as we said, is cumbersome. We could implement the same idea (measuring the distance between lattices from the functional distance between their associated functions) by means of another lattice quantity, which we have already seen in this work, the smoothed pair correlation function $g_2(r, \epsilon)$.

Based on this function we define the distance:

$$\rho_p(A, B; \epsilon) = \left(\int_1^\infty \mathrm{d}r |g_2^A(r, \epsilon) - g_2^B(r, \epsilon)|^p \right)^{1/p}. \tag{27}$$

As we have already stated, ρ_p is not a metric since g_2 does not fix a lattice uniquely and different lattices can have identical g_2's.

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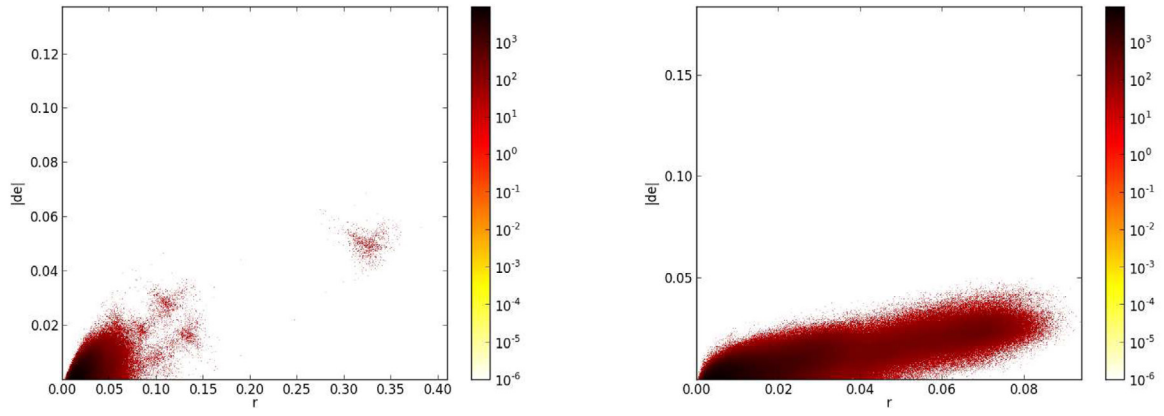


Figure 15. The scatter plot energy difference $|\delta e|$ versus lattice distance r, $d = 8$ (left) and $d = 13$ (right). The plots are generated from random subsets of extreme lattices of 1000 ($d = 8$) and 2000 ($d = 13$) lattices. The smoothing parameter used to compute the distances is $\epsilon = 0.1$.

Since we believe that as the dimension of the space increases, the knowledge of higher order correlations (g_3 etc) becomes less and less important (as stated by the *decorrelation principle*), we propose to trust that the distance between lattices given by (27) captures the 'geometrical distance' in a reasonable sense.

There are numerical issues: we can never compute the entire $g_2(r)$ for arbitrary distances and have to stop at some finite cutoff distance. However we have made sure that the smoothed g_2 is already close to its asymptotic value of 1 at these cutoff distances. We have also checked that the smoothing does not affect the results qualitatively.

We have studied correlations between energy difference $\delta e = |e(\Lambda) - e(\Lambda')|$ and inter-lattice distance $\rho(\Lambda, \Lambda')$ for extreme lattices by looking at the scatter plots for $d = 8$–13. The $d = 8$ and $d = 13$ are shown in figure 15. We see that lattices that are *equally dense* are also located very *close* in the space of lattices. Such behavior is not typical for frustrated systems, where local minima with equal energies are typically very different. It is intriguing whether this trend extends beyond $d \approx 20$–21, where all the known *de novo* algorithms for the best packing discovery start to experience problems with identifying the best (known) lattice packing. It is plausible that the behavior we observed in low dimensions, changes for $d \gtrsim 21$–22.

8. Conclusions and open questions

8.1. Conclusions of this preliminary study

In this paper, we have studied some statistical properties of extreme lattices generated by a randomized version of the Voronoi algorithm (supplemented with an eutaxy test).

For the first time, a large ensemble of non-equivalent extreme lattices in dimensions up to $d = 13$ has been analyzed with the tools of statistical physics. Our goal has been to attempt to identify a *typical* behavior of extreme lattices under measures of symmetry, decorrelation, kissing numbers and packing fractions and extract the trend, that

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could be continued in (much) higher dimensions. We studied both the distributions and correlations of these quantities (i.e. whether higher symmetry implies lower decorrelation or better packing fraction).

In order to do this, we had to introduce new measures (or new interpretations of existing quantities) of decorrelation and symmetry (packing fraction or kissing number are easily measured) and get a sufficient statistics to answer the questions. Concerning typical properties, we see that typical extreme lattices have better packing fractions and kissing numbers than perfect lattices (of the same dimension d), but no evident trend can be extracted from our analysis, contrary to what one could do for perfect lattices [22].

Regarding the symmetry of a lattice, we employ the size of its automorphism group. To tame the fast growth of this number, we define the *symmetry exponent* of a lattice as

$$s = \ln|\mathrm{Aut}(\Lambda)|/d.$$

We observe that typical lattices have comparatively *low* symmetry, both compared to the densest and to the least dense cases.

To measure the degree of decorrelation, we have proposed a distance ξ (measured in units of lattice spacing) within which all features of $g_2(r)$ are contained (within a certain approximation). This is done in (25). For $r > \xi$, g_2 is almost featureless (when properly smoothed as suggested in [41]). This distance is also related to the concept of order metric introduced in [62]. We see that this distance is correlated with the symmetry measure s, in the sense that lattices with larger symmetry groups typically have also larger ξ.

When studying the correlation between ξ and the packing fraction however we find that, although for typical extreme lattices there is a mild correlation between shorter ξ and larger packing fraction, there is no such correlation when looking at best packers and worst packers. The worst packers are *always* less decorrelated than either the typical extreme or the best packers.

We have also considered the issue of whether lattices close in density are also close in some intuitive distance in the space of lattices. For the latter, we have used ρ in (27), defined as the L_p-norm for the summable functions $h(r) = g_2(r) - 1$ (g_2 is intended as appropriately smoothed), which are easily computed. We found that close in packing fraction typically means close in distance, which is not the typical behavior of frustrated systems.

We have verified that the least dense of the extreme lattices is A_d in all dimensions and for all extreme lattices we have found. We have also seen how for $d \geqslant 9$ the least dense extreme lattice has considerably more symmetries that the most dense.

We had to limit our analysis to $d \leqslant 13$, as the generation of extreme lattices becomes difficult using our procedure. As shown in [20] more extreme lattices can be generated in $d \gtrsim 14$ with the compressing algorithm we mentioned in section 3 allowing to extend our results to $d > 13$.

8.2. Open problems

Since this is one of the first studies in this direction, we identify below a series of open problems which we think could lead to interesting investigations.

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As mentioned before we have found that the density of typical extreme lattices is larger than that of typical perfect lattices. Do typical extreme lattices provide (further) improvement of Minkowski bound?

Do the A_d and D_d lattices decorrelate slower than the typical extreme lattices in any d? Distinct lattices with similar packing fractions are close in the space of lattices (see figures 15), as we have discovered. Is this statement true in all dimensions? In studies of disordered systems we are familiar with the situation in which configurations close in energy are typically far in some appropriate distance (for example Hamming distance in the case of frustrated spin systems, or real distance in the case of Anderson localized particles). Could it be that a similar situation arises in high-dimensional lattices? What is the link with the theory of configurational glasses? [63] This is an important issue for our understanding of the packings in high dimensions that deserves further investigation.

We have seen a special case, $d = 13$, where the best packer is much more decorrelated than the corresponding best packers in $d = 12$ and 14. What is the fate of such exceptional dimensions as $d \to \infty$? That is, which of the scenarios proposed in [30] is realized for $d \to \infty$? Do the special dimensions vanish or do they persist?

The decorrelation properties of the lattices were extracted from the pair correlator g_2 only. Higher order correlation functions, like g_3 or g_4, are also important in the context of the decorrelation principle. A more stringent test is to check explicitly whether g_3 and g_4 (or any higher correlators) factorize into products of ρ, the number density of the lattice, and g_2. So far such test was only carried out for the 'ghost' RSA [31] and related processes [29], and certain determinantal point processes [33, 64], where all the correlators can be computed exactly. The fermionic point processes have the property of three- and higher- point correlation functions factorize in terms of g_2.

When studying the symmetries of (extreme) lattice packings, we used the simplest possible measure, s. There are other measures, which might provide additional information. For example, the A_d and D_d lattices have very large but simple in some sense symmetry groups, while the densest known lattices have symmetry groups that are small, compared to those of A_d/D_d, yet with a richer structure. Their *richness* is reflected in the *running time* of the algorithm that computes the groups. In fact, while computing the $\mathrm{Aut}(A_{20})$ is a matter of no time even on a typical desktop machine, the computation of the symmetry group of Λ_{20}, the densest known lattice in $d = 20$, requires days of computing time on the same machine. It would be interesting to analyze the symmetry properties of the packings and their correlations, based on the *computational complexity* of the algorithmic task of their determination.

Another interesting problem is how the symmetry of a typical packing is related to its decorrelation properties as $d \to \infty$. Our results for extreme lattices suggest that packings with lower symmetry decorrelate faster, although there are some counterexamples. It will be extremely interesting to check this statement with non-lattice sphere packings.

Finally, we have only looked at lattice packings. It is extremely appealing to study packings with many particles in the unit cell (i.e. periodic packings). We expect generally that decorrelation is stronger for periodic packings than for lattices in some fixed dimension based on an initial study [41], but such a conclusion has yet to be verified in any complete sense.

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Appendix A. Definition of metric in the space of lattices

We used a g_2 based metric to compute distances between lattices. Here we discuss possible alternatives and their drawbacks.

The most tempting way to estimate the inter-lattice distance is to use one of the many matrix distances for the lattice Gram matrices. However, this is not a correct definition, since a single lattice can be represented by many different Gram matrices (arithmetical equivalence). It is possible to amend the matrix distance and make it aware of the equivalences: We define a distance between two lattices Λ and Λ' as a minimum matrix distance over all equivalent representations of the two lattices:

$$\rho(\Lambda, \Lambda') = \min_{U,\, V \in \mathrm{SL}_d(\mathbb{Z})} \| U^t\, Q\, U - V^t\, Q'\, V \|^2 \tag{A.1}$$

where Q and Q' are the respective Gram matrices. The minimization takes into account all possible isometric copies of Λ and Λ'. This is the most straightforward definition of the distance, but it is not practical, since it requires double optimization over all the lattice automorphisms, and we are not aware of any implementation of this metric.

Similarly, any metric that requires the knowledge of a lattice theta series is going to be impractical. There exists an algorithm, which makes use of theory of modular forms [1, 53], to compute the entire theta series starting from a finite initial piece of the series for lattices with rational Gram matrices. The computation is, again, not simple: MAGMA computational algebra system has routines that are able to perform at least part of the computation but the complexity of such computation grows quickly with the number of dimensions, and already in as low as $d = 6$ the complexity can be quite high.

Yet another possible definition of distance between extreme lattices makes use of the Voronoi graph. The distance $\rho(\Lambda', \Lambda)$ is equal to the shortest path connecting the extreme lattices Λ' and Λ. The big disadvantage of this definition is that the Voronoi graph is only known up to $d = 8$. Computing the graph in higher dimensions is, at present, a challenging problem.

Appendix B. Some known automorphism groups of lattices

We give below the sizes $|\mathrm{Aut}|$ of the groups of automorphisms for the A_d and D_d lattices as well as the densest lattices in dimensions $d = 2$–14.

Table B1. The sizes of automorphism groups for the densest known lattices in $d = 2$–19 and $d = 24$. Unlike the cases of A_d and D_d, the growth is not monotonic but rather it shows irregular oscillations on an underlying growing trend.

A_2	12
$A_3 \sim D_3$	48
D_4	1152
D_5	3840
$E_6 \sim \Lambda_6$	103 680
$E_7 \sim \Lambda_7$	2903 040
$E_8 \sim \Lambda_8$	696 729 600
Λ_9	10 321 920
Λ_{10}	884 736
K_{11}	207 360
K_{12}	78 382 080
K_{13}	622 080
Λ_{14}	884 736
Λ_{15}	41 287 680
Λ_{16}	89 181 388 800
Λ_{17}	1486 356 480
Λ_{18}	159 252 480
Λ_{19}	23 592 960
Λ_{24}	8315 553 613 086 720 000
Q_{32}	207 360

The D_d family of lattices is defined as the set of integer points $\mathbf{x} \in \mathbb{Z}^{d+1}$, such that $\sum_i x_i = 0 (\mathrm{mod}\, 2)$ [1]. In $d = 3$, the D_3 lattice is the FCC lattice. The D_d family of lattices represents the densest lattices in $d = 3$, 4, 5.

The size of the automorphism group of A_d and D_d is [1],

$$|\mathrm{Aut}(A_d)| = 2(d+1)!\,, \tag{B.1}$$

$$|\mathrm{Aut}(D_d)| = 2^d d!\,, \tag{B.2}$$

(the only exception being D_4 with the size 1152 instead of 384 given by the above formula), giving the following asymptotic $d \to \infty$ behavior

$$s(A_d) \simeq \ln(d) - 1 + \mathrm{O}(\ln d/d), \tag{B.3}$$

$$s(D_d) \simeq \ln(d) + \ln(2) - 1 + \mathrm{O}(\ln d/d). \tag{B.4}$$

This means that these lattices have a superexponential growth of the size of their automorphism groups, while the best packers have relatively small sized groups, an indication that the decorrelation principle might be at work here.

Many of the densest lattices represented in table B1 belong to the so-called laminated family of lattices, which is is denoted as Λ_d [1]. The known exceptions are K_{11}, K_{12}, K_{13}. The laminated lattices are constructed in a recursive way, starting from $d = 1$. Their construction exploits a natural idea, that we can get a $d+1$ lattice Λ_{d+1} from a dense d-dimensional Λ_d by stacking layers of Λ_d in a smart way. Namely, we should place the spheres of the next layer in the *deep holes* of the current layer. The deep holes are the points of space that have maximal distance from any lattice point [1]. We illustrate this

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construction, by showing the first few steps of the recursion. In $d = 1$ there is a single lattice: it is simply a chain of touching spheres. In $d = 2$ we stack the layers, so that every next layer has its spheres shifted by half a lattice spacing with respect the previous layer. This generates the $\Lambda_2 \sim A_2$ hexagonal lattice. Repeating the procedure for the hexagonal lattice, we get the FCC lattice $A_3 \sim D_3$. Notice, that the construction outcome is not unique: it is easy convince oneself that there are uncountably many inequivalent ways to stack layers of A_2, all of them giving sphere packings of the same density as that of FCC lattice A_3. This is an important observation, since in higher dimension the construction procedure also generates many lattices, and one needs to pick the densest.

Appendix C. Generation of extreme lattices

We discuss in this section here possible alternatives to the algorithm, that was described in section 3 and that we used to find extreme lattices. There are several directions in which the original generation procedure can be altered.

One possibility is to restart the random walks many times and collect the statistics. However, we need an initial perfect lattice, that has to be generated by previous random walks as we presently do not have an algorithm to generate random perfect lattices without performing a random walk. As we have found numerically, there is little difference whether we restart the random walk (RW) many times or if we perform a single long random walk. Restarting many times only makes sense if combined with temperature bias towards denser lattices, i.e. we only accept lattices with higher density than the current one, with some probability, that depends on fictitious temperature [22]. However, we find that for higher temperatures there is little difference with normal RW, as was explained in [22]. For low fictitious temperature the random walk quickly reaches a local minimum and only explores its neighborhood, which appears to contain many equivalent copies of few extreme lattices.

Another idea, is to bias the random walk towards denser lattices, i.e. at every step choose the neighbor that has higher density. Unlike the Monte-Carlo mentioned above [22], in this algorithm it is the way the neighbor of the current lattice is picked is modified, so that denser lattices are preferred. Then, if the RW starts from some perfect lattice, always choosing the densest neighbor, the RW has to reach extreme lattice after a finite number of steps. The expected number of steps required to reach a local maximum is smaller than for a simple RW. Unfortunately, the test implementation of this algorithm has shown no improvement with respect to regular RW [55].

The most promising route is to use the sequential linear programming of [19], which was shown to generate large number of inequivalent extreme lattices in $d > 13$ [20].

It is also worth pointing out the connection between the algorithm of [22] and [19]. The former might be considered a variant of simplex method widely used to solve linear programs, while the latter corresponds to the interior point method also used in linear programming.

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