Statistical mechanics of the lattice sphere packing problem

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We present an efficient Monte Carlo method for the lattice sphere packing problem in d dimensions. We use this method to numerically discover *de novo* the densest lattice sphere packing in dimensions 9 through 20. Our method goes beyond previous methods, not only in exploring higher dimensions but also in shedding light on the statistical mechanics underlying the problem in question. We observe evidence of a phase transition in the thermodynamic limit $d \to \infty$. In the dimensions explored in the present work, the results are consistent with a first-order crystallization transition but leave open the possibility that a glass transition is manifested in higher dimensions.

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The problem of identifying the highest density sphere packing in d dimensions is a classical problem in geometry with direct connections to fields of physics, information theory, and mathematics. The case $d = 3$, for which Kepler conjectured that the face-centered cubic lattice is optimal, stood as an open problem for centuries before, finally, in 1998, a proof was announced by Hales [1]. Aside from dimensions 2 and 3, the highest density is not known in any other dimension, although it has been bounded to an extremely tight interval in dimensions 8 and 24 [2].

The highest packing densities that have been obtained in these dimensions, as in many others, are obtained by Bravais lattices: periodic packings with one sphere in each unit cell. From this point on, we use "lattice" to mean a Bravais lattice unless a nontrivial basis is mentioned. When restricting the sphere packing problem to lattices, many simplifications are possible, and the problem becomes more tractable, but still far from trivial. In fact, the densest lattice packings are known in dimensions $d \leqslant 8$ and $d = 24$ [2,3]. The space of lattice packings in d dimensions is finite-dimensional and much simpler to study than the infinite-dimensional space of all possible packings.

In fact, it is possible, in principle, to identify all local density maxima in this space. Such lattices, called extreme lattices, have been characterized by Voronoi in terms of their algebraic properties. Voronoi showed that a lattice is extreme if and only if it is perfect and eutactic [4]. Perfect lattices—those that are fully determined by a list of their shortest vectors—are finite in number, and Voronoi gave an algorithm that enumerates all the perfect lattices in a given dimension. In dimensions $d \leqslant 8$, the identity of the densest lattice packing has been established by an exhaustive enumeration of the perfect lattices. Voronoi's algorithm relies on a method of obtaining, starting from any perfect lattice, a set of *neighboring* perfect lattices. Voronoi showed that this graph of neighbors is connected, so exploring larger and larger neighborhoods of a single perfect lattice would eventually uncover all perfect lattices.

However, as the number of perfect lattices grows rapidly in dimensions $d > 8$, exhaustive enumeration becomes impractical, and other methods must be used to identify dense packings. Analytic constructions based on groups, codes, and laminated lattices have been successful in producing very dense lattice sphere packings in dimensions up to $d = 24$ and in certain dimensions above [3]. While these methods have certainly proved remarkably effective, they give little reason, on their own, to believe that they have, in fact, produced the densest possible structures.

For the latter purpose, in the absence of rigorous proofs (as in $d = 24$) or tight bounds, we rely on numerical methods that attempt to discover these structures *de novo*: without *a priori* knowledge of their existence. It is only recently that such methods were introduced that could tackle moderately high dimensions. A method based on the "divide and concur" framework for constraint satisfaction problems was used in Ref. [5] to discover *de novo* the densest known lattices in $d \leqslant 14$. In Ref. [6], Andreanov and Scardicchio implemented a random walk on Voronoi's graph, yielding a random sample of perfect lattices. While their method was designed to explore random perfect lattices and their statistics, they were also able to use it for *de novo* discovery of the densest lattice packing. In dimensions $8 \leqslant d \leqslant 12$, their random sample included the densest known lattice packing, while in dimensions $13 \leqslant d \leqslant 19$, they had to bias their random steps toward higher density configuration to recover the densest known packing. In $d = 19$, only some of these biased walks ended up visiting the densest known lattice. In Ref. [7], Marcotte and Torquato used a sequential linear programming (SLP) approach to iteratively compress a lattice configuration until it reaches a configuration that cannot be compressed any more—an extreme lattice. This procedure, starting from random initial conditions, reproduced the densest known lattice in an appreciable portion of the runs in each dimension $d \leqslant 16$. The percentage of runs yielding the densest known lattice declines sharply starting at $d = 17$. However, because each run can still be computed rapidly, the procedure can be repeated many times and the densest known lattice is produced at a decent rate for $d \leqslant 19$ (see below for a direct comparison with the present method). Other methods have been used for *de novo* searches in closely related problems, such as the Gaussian-core soft-sphere ground-state problem [8] and the lattice quantizer problem [9].

In this paper, we report on a Monte Carlo (MC) method for studying the lattice sphere packing problem. Our method is completely different from the references above, but some of our results are surprisingly similar to the results of Refs. [6,7]. In particular, in each dimension $d \leqslant 19$, a simulated quasistatic

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compression discovers *de novo* the densest known lattice in at least 30% of the runs. In 20 dimensions, only 1 of 50 quasistatic compression runs yielded the densest known lattice. However, with a slight change in protocol, we were able to reproduce the lattice in 7 of 50 runs. That three such disparate methods all seem to start having serious difficulties in the same dimensions raises the possibility that the lattice sphere packing problem becomes intrinsically harder around $d = 20$. We suggest possible reasons for such a scenario. Moreover, because of the statistical mechanical nature of our method, we are able to quantitatively characterize the intrinsic nature of the lattice sphere packing problem apart from the behavior of any specific method or algorithm for its solution.

A lattice can be specified by its generating matrix: the set of all sphere centers is given by $M^T\mathbb{Z}^d = \{M^T\mathbf{n} : \mathbf{n} \in \mathbb{Z}^d\}$, where M is a $d \times d$ matrix and its rows are generating vectors (primitive vectors) of the lattice. While a generating matrix uniquely specifies a lattice, a lattice has multiple generating matrices: whenever Q is a unimodular integer matrix, $M' = QM$ generates the same lattice as M. A lattice is a packing of radius-1/2 spheres (that is, its spheres do not overlap) if $||M^T\mathbf{n}||^2 \geqslant 1$ for all $\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}$. If this is the case, we say the lattice is *admissible*. The number density of spheres is given by $1/v = 1/|\det M|$, where v denotes the unit cell volume. Any lattice, generated by M, can be rotated so that its generating matrix MU, where U is a rotation matrix, becomes lower-triangular. Therefore, the space of lattices, modulo rotation, can be parameterized by lower-triangular generating matrices.

We can define an isobaric ensemble on the space of admissible lattices by weighting the probability of each lattice by a factor $\exp(-pv)$, where $p = NP/k_BT$ is a reduced pressure variable (cf. Ref. [10] for definitions of related ensembles). If v is thought of as the energy associated with a particular lattice, we can think of p as the inverse-temperature (cf. Ref. [6], where $\log v$ is used as the energy). We can sample this ensemble using a standard Metropolis algorithm: a random element of the lower-triangular generating matrix is randomly changed by a small amount; the step is rejected always if it yields an inadmissible lattice and is rejected with probability $\exp(-p\Delta v)$ if the unit cell volume is increased by Δv. However, we find instead that it is more efficient to build the detailed balance directly into the proposed steps instead of the acceptance probability. Note that changes to the off-diagonal elements of the matrix do not change the volume. Therefore, these moves are always accepted if they produce admissible lattices. For the diagonal elements, we propose changes

$$m_{ii} \leftarrow \left(1 + \frac{\epsilon x - \frac{1}{2}\epsilon^2 p}{v}\right) m_{ii},$$

where $v = \prod_{j=1}^{d} m_{jj}$ is the current volume, ϵ is a measure of the typical move size, and x is drawn from a normal distribution of unit variance. As with the off-diagonal moves, the proposed moves are always accepted if they produce admissible lattices. Note that the change in volume is given by $\Delta v = \Delta m_{ii} v/m_{ii} = \epsilon x - \frac{1}{2}\epsilon^2 p$ and is distributed with a probability density of

$$\frac{1}{\epsilon\sqrt{2\pi}} \exp\left[-\frac{\left(\Delta v + \frac{1}{2}\epsilon^2 p\right)^2}{2\epsilon^2}\right].$$

Therefore, an accepted move changing the volume by $\Delta v > 0$ is less likely by a factor of $\exp(p\Delta v)$ than the reverse move, as required by detailed balance.

A crucial step in this MC algorithm is checking whether a lattice is admissible. This is known to be an NP-complete problem [11], and in fact it takes up most of the computational time in our simulations. The complexity of this problem is sensitive to the choice of generating matrix for a given lattice. Generally speaking, the shorter and more orthogonal to each other the generating vectors are, the easier the problem is of determining admissibility of the lattice they generate. There are many nonequivalent criteria for determining how well-suited, or *reduced*, a certain set of generating vectors is. We use Korkine-Zolotareff (KZ) reduction, which is one of the most stringent of these criteria [12]. Such a stringent criterion is warranted because of the large number of times we are required to decide the admissibility of similar lattices. Therefore, during our simulation we periodically perform KZ reduction, and thus all the generating matrices we consider are either KZ-reduced or nearly so. Detailed balance is violated by these reductions, but we find that the reductions are rare enough in the key stages of the simulations that they do not significantly hinder thermalization.

Using our MC technique, we perform a simulated quasistatic compression (a simulated annealing where pressure takes the role of temperature). We start the system in a simple hypercubic lattice $\mathbb{Z}^d$ and equilibrate at a constant pressure. We then start to increase the pressure by a constant factor after each proposed move. We vary the typical move size inversely with the pressure: $\epsilon = \epsilon_0/p$. We use different move sizes for off-diagonal and diagonal moves, and for both we pick ϵ_0 so as to achieve an average move acceptance rate of roughly 30%. The length of the equilibration period is 4% of the length of the compression period. The Gram matrix $G = MM^T$ of the final matrix obtained in nearly all runs consists, up to small errors, of small-denominator rational numbers. Therefore, we can easily round off its entries to obtain the infinite pressure limit of the simulation.

For each dimension $d = 9, \ldots, 19$, we performed 20 simulation runs. In each of these dimensions, our simulations discover the densest known lattice packing in at least 30% of the runs. Table I summarizes the results of these simulations. The compression rate used represents a trade-off between longer computation time and decreased likelihood of reproducing the densest lattice. We did not attempt to quantify this trade-off in this paper or determine the optimal compression rate as a function of dimension. In terms of the average computational time needed to reproduce the densest known lattice once, the present method is much less efficient than the SLP method of Ref. [7] in all lower dimensions. For the highest dimensions, $d = 17, 18$, and 19, respectively, this average time is 3×10^3s, 8×10^4s, and 2×10^6s with the SLP method, compared to 2×10^5s, 3×10^5s, and 8×10^5s with the present method.

Assuming our MC simulations accurately sampled the isobaric ensemble at each pressure, we would recover from the simulation the equation of state: the average volume $\langle v \rangle$ as a function of the reduced pressure p. Plotting the traces of $\langle v \rangle$ as a function of p for different runs in dimension $d = 11$, for example (Fig. 1), we see that at a certain pressure the different traces diverge and the simulations fall out of

TABLE I. For each dimension d, the table gives the following: the name (as per Refs. [3,13]) of the lattice Λ that achieves the greatest density known among all admissible lattices; the unit cell volume v of this lattice (normalized by 2^d); the reduced pressure p_i used in the equilibration period and at the beginning of the compression period of our simulations; the reduced pressure p_f at which we terminated the compression; the compression rate k, such that the pressure at each proposed move is $1 + k$ times the pressure at the previous proposed move; the average computational time T per run of the simulation; and the rate at which the lattice Λ is reproduced, that is, the percentage of runs whose final configuration, after rounding off the Gram matrix, is Λ.

d	Λ	$2^d v$	p_i	p_f	k	T (sec.)	Rate
9	Λ_9	$16\sqrt{2}$	20	2×10^4	1.4×10^{-6}	60	1
10	Λ_{10}	$16\sqrt{3}$	60	6×10^4	1.4×10^{-6}	1.2×10^2	1
11	K_{11}	$18\sqrt{3}$	2×10^2	2×10^5	4.6×10^{-7}	7.8×10^2	0.55
12	K_{12}	27	3×10^2	3×10^5	6.9×10^{-7}	1.1×10^3	1
13	K_{13}	$18\sqrt{3}$	6×10^2	6×10^5	3.5×10^{-7}	3.0×10^3	0.70
14	Λ_{14}	$16\sqrt{3}$	2×10^3	2×10^6	1.8×10^{-7}	9.4×10^3	0.60
15	Λ_{15}	$16\sqrt{2}$	3×10^3	3×10^6	3.5×10^{-7}	9.1×10^3	0.90
16	Λ_{16}	16	5×10^3	5×10^6	1.8×10^{-7}	2.9×10^4	0.95
17	Λ_{17}	16	1.5×10^4	1.5×10^7	6.9×10^{-8}	1.2×10^5	0.8
18	Λ_{18}	$8\sqrt{3}$	7×10^4	1.8×10^7	5.5×10^{-8}	1.9×10^5	0.6
19	Λ_{19}	$8\sqrt{2}$	9×10^4	2.2×10^7	4.6×10^{-8}	2.4×10^5	0.3
20	Λ_{20}	8	3×10^5	8.2×10^6	3.5×10^{-8}	3.3×10^5	0.14

equilibrium. The traces belonging to runs that terminate at the same configuration do not diverge, so we may infer that at this pressure the system goes from exploring the attraction basins of many different extreme lattices to exploring only a single basin. The situation becomes more complicated in higher dimensions, where we see significant hysteresis effects. For example, in dimension $d = 16$, all 20 runs end up in the basin of the densest known lattice Λ_{16} (Fig. 1), but different runs experience the transition at different pressures. Figure 2 shows, for each dimension, the volume as a function of pressure averaged over all the runs that yielded the densest known packing.

For any fixed d, as there is no thermodynamic limit, strictly speaking, there cannot be a phase transition. However, as is clear from Figs. 1 and 2, the system shifts as the pressure increases from a state where many basins of attraction are explored to a state where the system is confined to a single basin. In any finite dimension there should be a range of pressure where these two states coexist with significant probability for the system to be in either state. The traces we obtain from the simulations are consistent with a situation where the transition rate between these two states in the coexistence region becomes smaller and smaller with increased dimension, so that in lower dimensions the trace of each run remains close to the equation of state, while in higher dimensions each run stays in one state until transitioning irreversibly into the other. This crystallization transition is accompanied by a discontinuity in the density, which depends on the extreme lattice the system crystallizes into.

We may interpret $d \to \infty$ as the thermodynamic limit of the lattice sphere packing problem and speculate that the coexistence region in this limit shrinks to a single critical pressure. Parisi considers the partition function of a closely related ensemble of lattices in the limit $d \to \infty$ and points out that the lattice sphere packing problem in this limit shares many formal similarities with the nonlattice problem [10]. Parisi does not determine whether a glass transition exists in the lattice sphere packing problem as it does in nonlattice hard sphere system and leaves open the possibility of either a glass transition or a crystallization transition. The behavior we observe in our simulations in dimensions $9 \leqslant d \leqslant 19$ is indicative of a first-order crystallization transition. However, it is hard to tell whether the behavior is controlled by the thermodynamic limit or mostly by details specific to the moderate dimensions we explore.

In dimension $d = 20$, out of 50 runs at the slowest compression rate attempted, only one yielded the densest known lattice. In fact, only ten runs show a discontinuity in the density at all, with most runs remaining in the fluid state throughout. In another set of 50 runs, we compressed to an intermediate pressure, where we expect the crystallization rate to be higher, and maintained that pressure until we observed a rapid increase in density. With this new protocol, the densest lattice is reproduced in seven runs.

We find it remarkable that both our method and the methods of Refs. [6,7] become dramatically less effective at exactly the same dimension. Whereas *a priori* we might expect that the complexity of the lattice sphere packing problem rises at a more or less constant exponential rate as a function of dimension, the evidence of the two cited works and the present paper raises the hypothesis that the complexity experiences a sharp increase around $d = 20$. A sharp increase of this kind might indicate a shift into the glassy regime of the lattice sphere packing problem. Just as the relaxation time of a fluid increases sharply as the glass temperature is crossed, it might be the case here that $d \approx 20$ marks the beginning of a glassy regime, linked to a sharp increase in the inverse compression rate required to recover the densest lattice.

In addition to discovering *de novo* the densest known lattice in dimension d, our method can also be used to discover suboptimal, yet very dense, extreme lattices. In some dimensions, only a portion of runs, even at the slowest compression rate attempted, yielded the densest known lattices (see Table I). The identity of the suboptimal lattices produced is in some

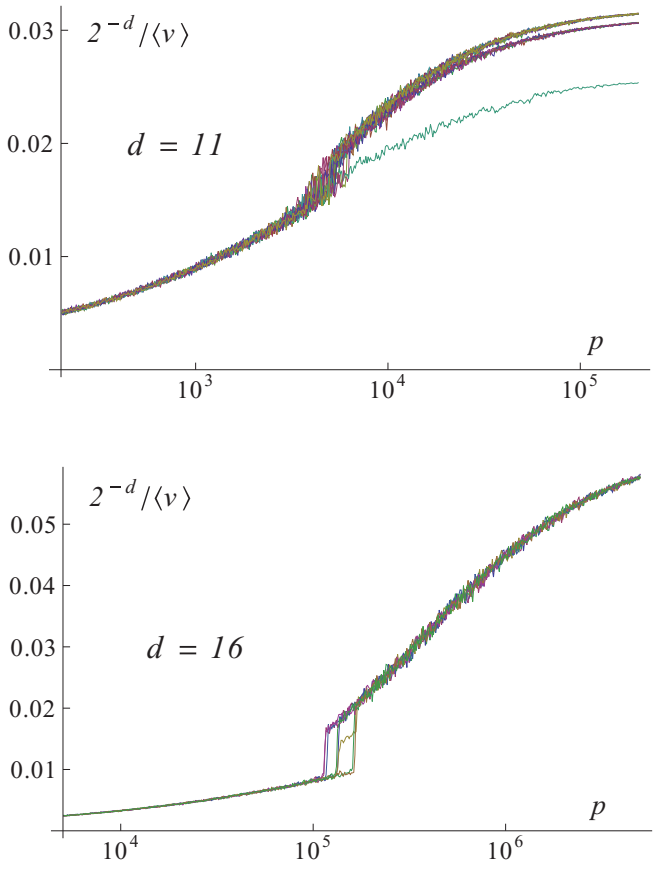

FIG. 1. (Color online) Traces of density as a function of reduced pressure in different runs in dimensions $d = 11$ and $d = 16$. In 11 dimensions, the simulation remains in equilibrium until around $p = 4.8 \times 10^3$, where different runs continue along different branches, corresponding to basins of attractions of different extreme lattices. In 16 dimensions, all runs end up in the basin of the same lattice, but we observe that different runs make the transition into this basin at different pressures. It appears that at least one of the runs also spends some time in an intermediate state, presumably the basin of attraction of a different extreme lattice.

cases unexpected, and the second-most-likely-produced lattice is not always the second-densest known extreme lattice. For example, in dimension $d = 14$, the most frequently produced lattice after Λ_{14} in our simulations is a lattice (denoted "dim14kis744" in Ref. [13]) of normalized unit cell volume $2^{14}v = 361\sqrt{3}/16$, compared to $2^{14}v = 16\sqrt{3}$ for Λ_{14}. This is also the second-densest lattice produced, despite the existence of many extreme lattice of intermediate density [7]. As was already observed in the results of Ref. [7], we observe a general trend wherein among extreme lattices of equal density, those with lower kissing numbers (number of neighbors in the first coordination shell) are more frequently produced, though this

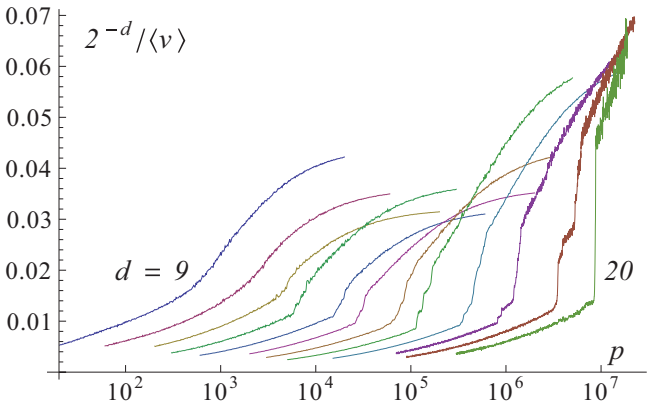

FIG. 2. (Color online) Traces of (normalized) density as a function of reduced pressure, averaged over all quasistatic compression runs that yielded the densest known lattice in each dimension $d = 9, \ldots, 20$.

trend is not without exceptions. In the present context, it makes sense that at finite pressures the basin of an extreme lattice with a lower kissing number is stabilized by a greater rattling entropy over the basin of another extreme lattice of equal density and higher kissing number.

Many of the lattices discovered by our simulations have not, to our knowledge, been studied before, and we have submitted them to be archived in the online catalog of lattices [13]. A few in particular are definitely worthy of further study. For example, one of the lattices we discover in dimension $d = 11$ (denoted "dim11kis422" in Ref. [13]) is equal in density to the two laminated lattices $\Lambda_{11}^{\min,\max}$. Remarkably, the lattice does not include any of the laminated lattices Λ_d for $d = 8,9,10$ as sublattices of equal minimum norm. This discovery suggests a possible extension to the conventional lamination hierarchy described in Refs. [3,14,15].

While the focus of the present paper is limited to the lattice sphere packing problem, the method presented can easily and naturally be extended to study lattices with an n-element basis for $n > 1$. The smallest dimension in which the densest known packing has a nontrivial basis is $d = 10$, where it has a 40-element basis [3]. In higher dimensions, there are known packings with more modest basis sizes (for example $n = 4,3$ in dimensions $d = 20,22$, respectively [16]) that are denser than the densest known lattices. Extending our capabilities to the point of being able to discover *de novo* any of these nonlattice structures or the densest known lattices up to $d = 24$ would be a major accomplishment. Of course, discovering yet unknown lattice and nonlattice packings denser than those constructed analytically should be considered the ultimate goal.

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