

Counterintuitive ground states in soft-core models

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It is well known that statistical mechanics systems exhibit subtle behavior in high dimensions. In this paper, we show that certain natural soft-core models, such as the Gaussian core model, have unexpectedly complex ground states even in relatively low dimensions. Specifically, we disprove a conjecture of Torquato and Stillinger, who predicted that dilute ground states of the Gaussian core model in dimensions 2 through 8 would be Bravais lattices. We show that in dimensions 5 and 7, there are in fact lower-energy non-Bravais lattices. (The nearest three-dimensional analog is the hexagonal close-packing, but it has higher energy than the face-centered cubic lattice.) We believe these phenomena are in fact quite widespread, and we relate them to decorrelation in high dimensions.

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I. INTRODUCTION

One of the most natural soft-core models in statistical mechanics is the Gaussian core model (introduced by Stillinger [1]), in which identical particles interact via a repulsive Gaussian pair potential. This is not only a beautiful theoretical model, but also a reasonable model for the effective interaction (via entropic repulsion) between the centers of mass of two polymers, namely, the Flory-Krigbaum potential [2,3]. Much work has gone into characterizing the phase diagram and ground states of the Gaussian core model [4,5].

We use the Gaussian core model as a test case for studying the emergence of long-range structure in classical ground states. In two or three dimensions, these ground states are typically lattices, and even Bravais lattices. The theory behind this phenomenon is poorly understood: the Lennard-Jones potential in two dimensions has been rigorously analyzed by Theil [6], and Sütő [7,8] has analyzed potential functions whose Fourier transforms are nonnegative and have compact support, but for no purely repulsive soft-core potential in more than one dimension is there a compelling argument for crystallization (let alone a proof). In the present paper, we show the subtlety of this problem by exhibiting counterintuitive ground states with different structure than anticipated.

Specifically, we study the Gaussian core model for dilute systems in high-dimensional spaces. Although that may sound arcane, such systems play an important role in statistical physics. First, they include sphere packing problems as a limiting case. Packing in high dimensions is of fundamental importance in communication and information theory, because (as Shannon discovered) finding codes for efficient communication in the presence of noise amounts to a packing problem in the high-dimensional space of possible signals.

Second, such systems provide an intriguing test case for the decorrelation effect, a fundamental phenomenon predicted by Torquato and Stillinger [9]: in loose terms, unconstrained spatial correlations should vanish asymptotically in high dimensions, and all multibody correlations will be reducible to the pair correlation function. Although it seems difficult to justify rigorously, decorrelation leads to surprising conjectures such as the existence of extraordinarily dense disordered packings in high dimensions (with important implications in information theory). See also Ref. [10] for a replica symmetry-breaking approach to amorphous packings in high dimensions.

This line of reasoning suggests that glassy states of matter are intrinsically more stable than crystals in high dimensions, which stands in stark contrast to intuition derived from most two- or three-dimensional systems. In three dimensions, for example, the low-density ground state for the Gaussian core model is the face-centered cubic (fcc) lattice, which has lower energy than the competing hexagonally close-packed (hcp) lattice, let alone disordered structures. In the present paper, we show that the opposite happens in as few as five dimensions: relatively exotic non-Bravais lattices improve on more familiar structures. To find this behavior in such a low dimension is unexpected, and while we cannot demonstrate the full decorrelation effect (for example, with completely amorphous packings), our results show that the role of order and structure in even low-dimensional ground states is more subtle than was previously realized.

Our direct motivation is a recent prediction by Torquato and Stillinger [11] for the ground states of the Gaussian core model in moderately high dimensions (up through \mathbb{R}^8 and also \mathbb{R}^{24}). Specifically, at sufficiently low particle density, they conjectured that the ground states are the Bravais lattices corresponding to the densest known sphere packings, and at sufficiently high particle density they conjectured that the ground states were the reciprocal Bravais lattices. In the case of \mathbb{R}^2 , \mathbb{R}^8 , and \mathbb{R}^{24} , this agrees with an earlier conjecture of Cohn and Kumar (conjecture 9.4 in Ref. [12]). Zachary, Stillinger, and Torquato [13] have given strong numerical evidence that these are indeed the true ground states among

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known families of Bravais lattices. However, in this paper we disprove Torquato and Stillinger’s conjecture by exhibiting non-Bravais lattices with lower energy in the low density limit in \mathbb{R}^5 and \mathbb{R}^7 .

These improved lattices in fact correspond to tight sphere packings (i.e., sphere packings that are not only as dense as possible globally, but also locally, in the sense that there are no missing spheres, small gaps, etc.). Conway and Sloane [14] provided a conjecturally complete list of tight packings in low dimensions, and our ground states can be found in their list. They stand in the same relationship to the optimal Bravais lattices as the hcp packing stands to the fcc packing in \mathbb{R}^3 , but the energy comparisons work out notably differently. This is in effect another facet of decorrelation. Even within the restrictive class of tight packings, in high dimensions Bravais lattices are no longer energetically favored. Instead, somewhat less regular structures are preferred.

For comparison to the mathematical literature (and, in particular, Ref. [14]), note that mathematicians use “lattice” to mean “Bravais lattice” and “periodic packing” to mean “lattice with a basis.” In this paper, we follow the physics terminology.

II. THETA SERIES

All of our work in this paper takes place in the low density limit. Because of the scaling invariance of Euclidean space, we can instead fix the particle density and rescale the Gaussian. Specifically, we use the potential function $V(r) = e^{-\alpha r^2}$ between two particles at distance r , and we let α tend to infinity, which corresponds to taking the low-density limit.

The theta series for a packing \mathcal{P} (i.e., a collection of particle locations) is a generating function that describes the average number of particles at a given distance from a particle in \mathcal{P} . Specifically,

$$\Theta_{\mathcal{P}}(q) = \sum_r N_r q^{r^2},$$

where the sum is over all distances r between points in the packing, N_r denotes the average over all $x \in \mathcal{P}$ of the number of $y \in \mathcal{P}$ such that $|x-y|=r$, and q is a formal variable. The use of r^2 rather than r in the exponent is traditional in mathematics. Note that the theta series encodes the same information as the pair correlation function; we use this notation since it is convenient for the Gaussian core model.

Under the Gaussian core model potential function $V(r) = e^{-\alpha r^2}$, the average energy per point in \mathcal{P} equals $(\Theta_{\mathcal{P}}(e^{-\alpha}) - 1)/2$. (We subtract 1 to correct for the $r=0$ term in the theta series, which would correspond to a self-interaction, and we divide by 2 to avoid double counting.) Thus, computing theta series is exactly the same as computing energy in the Gaussian core model. The limit as $\alpha \rightarrow \infty$ of energy corresponds to the limit as $q \rightarrow 0$ of the theta series.

Given two packings with the same density (i.e., the same number of particles per unit volume in space), we can easily compare their behavior in the $q \rightarrow 0$ limit. Suppose their theta series are

$$\Theta_1 = 1 + a_{r_1} q^{r_1^2} + a_{r_2} q^{r_2^2} + \dots$$

and

$$\Theta_2 = 1 + b_{s_1} q^{s_1^2} + b_{s_2} q^{s_2^2} + \dots$$

with $r_1 < r_2 < \dots$ and $s_1 < s_2 < \dots$. To compare Θ_1 with Θ_2 , we need only consider the first term at which they differ. If $r_1 > s_1$, then $\Theta_1 < \Theta_2$ for small q ; if $r_1 = s_1$, then the comparison amounts to whether $a_{r_1} < b_{s_1}$. If $r_1 = s_1$ and $a_{r_1} = b_{s_1}$, then we must proceed to the next term.

Corresponding to any point configuration in \mathbb{R}^n , we obtain a sphere packing by centering identical spheres at the points of the configuration, with the maximal possible radius subject to avoiding overlap. The density of the packing is the fraction of space covered. To avoid confusion, we will distinguish between the particle density (the number of particles per unit volume in space) and the packing density (the fraction of space covered by balls).

As pointed out above, maximizing packing density is a consequence of minimizing energy in the Gaussian core model in the $\alpha \rightarrow \infty$ limit (with fixed particle density): the dominant contribution to the Gaussian energy comes from the smallest distance between points, which is large exactly when the packing density is large. In other words, the problem of maximizing the sphere packing density arises naturally as the low-density limit of the Gaussian core model.

III. TIGHT PACKINGS

In most dimensions, the sphere packing problem exhibits high degeneracy, in the sense that there are many geometrically distinct, optimal solutions (such as in three dimensions, with the fcc and hcp packings and their relatives). Conway and Sloane [14] gave a conjectural classification of all the tight packings in low dimensions. Here, tight means roughly that the global density is maximized and furthermore no local changes can add more spheres. (For example, removing one sphere from a dense packing leaves the global density unchanged, but the result is no longer tight.) The precise definition of tightness in Ref. [14] is problematic; see Ref. [15] for details on the problem and better definitions. Because they recognized that their definition was only tentative, Conway and Sloane characterized tightness by articulating “postulates” that they felt a correct definition should satisfy. These postulates are by no means obvious statements; instead, they are empirical observations from Conway and Sloane’s study of the packing problem.

Conway and Sloane [14] postulate that, in dimensions up to 8, every tight packing fibers over a tight packing whose dimension is the previous power of 2. To say that a packing \mathcal{P} fibers over \mathcal{Q} means that \mathcal{P} can be decomposed into parallel layers lying in $\dim(\mathcal{Q})$ -dimensional subspaces, each of which is a packing isometric to \mathcal{Q} . (In fact, in tight packings of dimensions up to 8 it will be a translate of \mathcal{Q} .) The locations of these parallel subspaces should themselves be determined by another tight packing. Although the Conway and Sloane postulates are only conjectures, they seem likely to be true and in this paper we assume their truth (but we note which ones are required for each theorem).

IV. DIMENSIONS UP TO 4

In \mathbb{R}^1 , there is exactly one tight packing, namely that given by the integers. It is provably optimal for the Gaussian core model by proposition 9.6 in Ref. [12].

In \mathbb{R}^2 , the triangular lattice A_2 is the only tight packing. Montgomery [16] showed that it is optimal among all Bravais lattices for the Gaussian core model, and it was conjectured in Ref. [12] that it is optimal among all lattices.

In \mathbb{R}^3 , all tight packings fiber over the triangular lattice A_2 . In other words, they are formed by stacking triangular layers, with the layers nestled together as densely as possible; each additional layer involves a binary choice for how to place it relative to the previous layer. These are the Barlow packings (i.e., the stacking variants of the fcc and hcp packings). It is not hard to check that, among these packings, the face-centered cubic lattice minimizes energy in the Gaussian core model in the low particle-density limit. This is consistent with the conjecture in Ref. [11].

In \mathbb{R}^4 , there is only one tight packing, namely the D_4 or checkerboard lattice (it is shown in Ref. [14] that only one tight packing fibers over A_2). It is defined to be the set of all integral points whose coordinates have even sum:

$$D_4 = \left\{ x \in \mathbb{Z}^4 : \sum_{i=1}^4 x_i \equiv 0 \pmod{2} \right\}.$$

The uniqueness of D_4 is remarkable, compared with the diversity of tight packings in \mathbb{R}^3 , and the D_4 lattice plays a fundamental role as a building block for higher-dimensional structures. It also appears that, much like the triangular lattice, D_4 may be universally optimal, in the sense that it is the ground state of the Gaussian core model at any density.

V. DIMENSION 5

In \mathbb{R}^5 , every tight packing fibers over D_4 , with the distance between successive layers being 1. To specify such a packing, one need only specify how each four-dimensional layer is translated relative to its neighbors. The deep holes in D_4 (the points in space furthest from the lattice) are located at $(1, 0, 0, 0)$, $(1/2, 1/2, 1/2, 1/2)$, and $(1/2, 1/2, 1/2, -1/2)$, as well as of course the translates of these points by vectors in D_4 . Each layer of a tight packing in \mathbb{R}^5 must either be an untranslated copy of D_4 or be translated by one of these vectors, so that the distance between layers is minimized; furthermore, adjacent layers must be translated by different vectors. In other words, the spheres in each layer must be nestled into the gaps in the adjacent layers.

If we let a denote the translation vector $(0, 0, 0, 0)$, b denote $(1, 0, 0, 0)$, etc., then each layer must be translated by one of $a, b, c,$ or d , and no two adjacent layers can be translated by the same vector. In other words, a tight packing in \mathbb{R}^5 is specified by a four-coloring of the integers (if we treat $a, b, c,$ and d as “colors”).

For example, the D_5 packing, which is the Bravais lattice with the highest packing density, corresponds to the following coloring:

$$\dots \textcircled{a} \textcircled{b} \textcircled{a} \textcircled{b} \textcircled{a} \dots$$

Note that the symmetries of the D_4 lattice arbitrarily permute $a, b, c,$ and d , so the choice of labeling is irrelevant. For D_5 , all that matters is that the layers alternate between two colors.

Conway and Sloane found that four tight packings are uniform, in the sense that all spheres play the same role (rather than the less symmetric situation of having several inequivalent classes of spheres). In addition to $D_5 = \Lambda_5^1$, the three others correspond to the following patterns:

$$\Lambda_5^2 : \dots abcdabcd \dots,$$

$$\Lambda_5^3 : \dots abcabc \dots,$$

$$\Lambda_5^4 : \dots bacbdcadbacbdcad \dots.$$

These three additional lattices are not Bravais lattices, but rather lattices with bases.

One can calculate that the theta series for Λ_5^1 is $1 + 40q^2 + 90q^4 + 240q^6 + \dots$, while the theta series of Λ_5^2 is $1 + 40q^2 + 88q^4 + 16q^5 + \dots$. It follows that Λ_5^2 has lower energy than D_5 in the $q \rightarrow 0$ limit, which disproves Torquato and Stillinger’s conjecture. In fact, the situation is even worse for D_5 , which is not only suboptimal but in fact the worst tight packing of all.

Theorem 1. Under postulates 2, 4, and 5 of Ref. [14], the Bravais lattice D_5 has the highest energy among all the tight five-dimensional lattices, in the $q \rightarrow 0$ limit.

To complete this calculation, we require four geometrical facts about D_4 . Specifically, each lattice point has 24 neighboring lattice points at squared distance 2, the next closest lattice points are 24 more at squared distance 4, each deep hole has 8 neighboring lattice points at squared distance 1, and the next closest lattice points to a deep hole are 32 points at squared distance 3. These assertions are easily checked by a short calculation.

Proof. Let Λ be a tight five-dimensional lattice, obtained by a four-coloring of the integers. We first observe that every sphere in Λ must have 40 neighbors at squared distance 2, for the following reason. Without loss of generality, we may assume that layer 0 is colored a and layer 1 is colored b (since the different deep holes are equivalent under the symmetries of D_4). Now, layer -1 cannot be colored a either, so the layers 0, 1, and -1 contribute $24 + 8 + 8 = 40$ neighbors of a given sphere in layer 0. (Every sphere in D_4 has 24 neighbors, which accounts for the 24 from layer 0, and each deep hole in D_4 is at distance 1 from 8 points of D_4 .) Therefore the theta series of Λ must start with $1 + 40q^2 + \dots$.

The next smallest possible squared distance in Λ is 4 (squared distance 3 does not occur in D_4 , and it cannot occur between adjacent layers since that would amount to having a lattice point at squared distance 2 from a deep hole). There are 24 spheres at that distance in D_4 , and 32 in each of layers ± 1 , for a total of 88. The only way there can be more is if they come from layers ± 2 , and each of those layers contributes one sphere (lying over the origin) if and only if it is colored the same as layer 0. Since D_5 corresponds to the

coloring $\cdots abababa \cdots$, its theta function has the maximum contribution to the q^4 term, making it the worst for energy as $q \rightarrow 0$. Furthermore, among all tight lattices only D_5 maximizes that term, so it is the unique pessimum. ■

The lattice Λ_5^2 turns out to be the best.

Theorem 2. Under postulates 2, 4, and 5 of Ref. [14], the lattice Λ_5^2 has the lowest energy among all the tight five-dimensional lattices, in the $q \rightarrow 0$ limit.

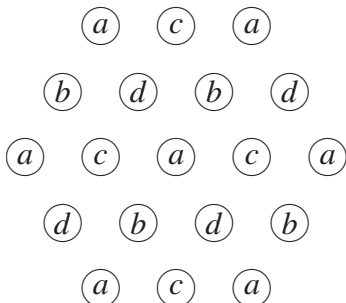
Proof. The proof is similar to that of the previous theorem. Let Λ be a tight packing as above, fibered over D_4 . We may assume as before that layer 0 is colored a . The first two terms of the theta series of Λ are 1 and $40q^2$. Now, if layer 2 or layer -2 were colored a , then Λ would have a larger q^4 term than Λ_5^2 , making it worse for potential energy in the $q \rightarrow 0$ limit. Therefore we may assume neither 2 nor -2 is colored a . The theta series is now determined up to the q^8 term, and it equals $1+40q^2+88q^4+16q^5+192q^6+64q^7+152q^8+\cdots$.

The q^9 term is not yet determined, since it depends on layers 3 and -3 . Merely being three layers apart contributes 3^2 to the squared distance, so they contribute to the q^9 term if and only if they are colored a . Thus, to minimize energy they must not be colored a . In other words, two layers of the same color must be separated by at least 4. The only way to do this is to color the layers $\cdots abcdabcd \cdots$, up to permutations of the four colors. Since permuting the four colors will not change the resulting lattice (because of the symmetries of D_4), we see that Λ_5^2 is the unique best lattice among all the tight five-dimensional lattices in the $q \rightarrow 0$ limit. ■

VI. DIMENSION 6

In \mathbb{R}^6 , the way to form tight packings is again to fiber over D_4 , and we must use the triangular lattice A_2 to arrange the fibers (with A_2 normalized so the closest lattice points are at distance 1). Thus, we are looking for four-colorings of the triangular lattice A_2 , where the colors specify which translation vector to use for the copy of D_4 . As in the previous dimension, the separation between adjacent layers will be 1.

The E_6 lattice, which is the Bravais lattice with the highest packing density, is given by the following coloring:



The theta series of E_6 is $1+72q^2+270q^4+936q^6+2160q^8+\cdots$. As shown by Conway and Sloane, there are three other uniform packings, corresponding to the following possibilities for the six neighbors surrounding a central a :

$$\Lambda_6^2 : bcbdbc,$$

$$\Lambda_6^3 : bcbcbc,$$

$$\Lambda_6^4 : bcbcbd.$$

In contrast to the five-dimensional case, the Bravais lattice E_6 is in fact optimal among all tight lattices in the $q \rightarrow 0$ limit.

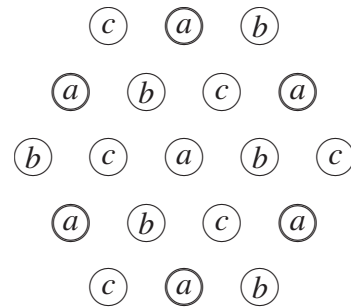
Theorem 3. Under postulates 2, 4, and 6 of Ref. [14], the Bravais lattice E_6 has the lowest energy among all the tight six-dimensional lattices, in the $q \rightarrow 0$ limit.

Proof. Let Λ be a tight packing formed as above by four-coloring the triangular lattice. Let us assume that the central sphere is colored a . The squared distances in the A_2 lattice are 1,3,4,..., so neighbors at squared distance 2 in Λ can come only from the central layer and its six adjacent layers. The number of these vectors is $24+6\cdot 8=72$, which is in accordance with the theta function of E_6 . The next possible squared distance is 3. Note that this distance does not occur in E_6 , since in the coloring above, there are no two spheres at squared distance 3 which have the same color. But in fact, the coloring above is the only coloring with this property (up to a permutation of the colors a, b, c, d , of course, but that is irrelevant because of the symmetries of D_4). To see this, start with the central sphere colored a , and notice that the six spheres around it must be colored $bcbdbc$ (or $bdcdbc$) to avoid two spheres of the same color being $\sqrt{3}$ units apart. One can then apply the argument to the six spheres centered around one of these six neighbors and proceed outward, to arrive at a unique packing: namely, the one above. This shows that E_6 is indeed the best for energy in the $q \rightarrow 0$ limit, among all tight lattices. ■

One can also determine the worst tight packing.

Theorem 4. Under postulates 2, 4, and 6 of Ref. [14], the lattice Λ_6^3 has the highest energy among all the tight six-dimensional lattices, in the $q \rightarrow 0$ limit.

We omit the details of the proof. However, the calculation amounts to showing that the Λ_6^3 coloring maximizes the number of identically colored spheres at squared distance 3 in A_2 . In the following picture of the coloring, the six bold circles are at squared distance 3 from the central circle:



VII. DIMENSION 7

Finally, in dimension 7 the optimal Bravais lattice E_7 is neither the worst nor the best for energy among tight packings in the low particle-density limit. According to Ref. [14], each tight packing in \mathbb{R}^7 fibers over D_4 , and the four-dimensional layers are arranged using a tight packing in \mathbb{R}^3 with adjacent D_4 layers separated by 1. To specify a four-coloring of the three-dimensional packing, we need only

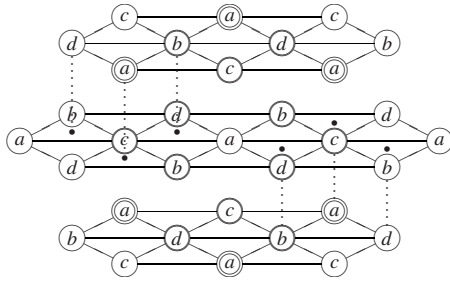


FIG. 1. The four-coloring of the fcc lattice used to obtain E_7 .

specify it on a single triangular layer, since each such layer determines the colors on both adjacent layers and hence on every layer.

We cannot use an arbitrary four-coloring of the triangular layer, since some colorings do not extend consistently to the other layers. Conway and Sloane showed that the condition for extending consistently is that the coloring should have “period 2” in the following sense: the packing should decompose into parallel strings of adjacent spheres, so that in each string the colors alternate between two possibilities. For example, the E_6 coloring shown in the previous section has this property (the strings lie along horizontal lines), while the Λ_6^3 coloring does not.

To obtain E_7 , we use the face-centered cubic as our tight packing in \mathbb{R}^3 , and we use the same coloring of a triangular layer as was used to construct E_6 . We get the picture in Fig. 1, which shows three triangular layers of the fcc lattice surrounding a central ball colored a (the dotted lines show how the layers are aligned, and the different styles of circles are for reference in the argument below).

The theta series of E_7 is $1 + 126q^2 + 756q^4 + \dots$, and we can see the first nontrivial term as follows. A point in the D_4 layer corresponding to the central circle colored a above has 24 neighbors at squared distance 2 in the same D_4 layer, 12·8 in neighboring D_4 layers (8 each from the 12 neighbors in the face-centered cubic, which have bold circles in Fig. 1), and 6 from non-neighboring D_4 layers (1 each from the 6 points in the face-centered cubic at squared distance 2, which are shown with two nested circles in Fig. 1 and are each colored a).

To improve upon E_7 in the $q \rightarrow 0$ limit, we can use the Λ_6^2 coloring of a triangular layer; the resulting tight packing is called Λ_7^3 . One can see from Fig. 2 that among the final six points in the calculation above, only four share the same

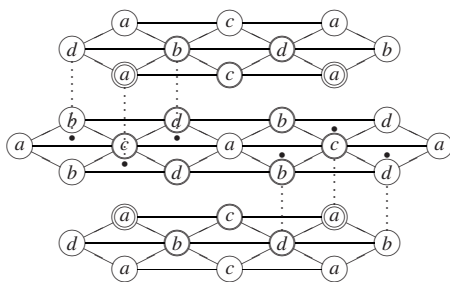


FIG. 2. The four-coloring of the fcc lattice used to obtained Λ_7^3 .

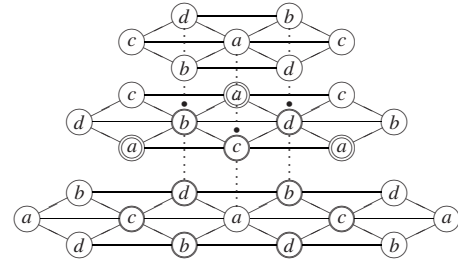


FIG. 3. The four-coloring of the hcp lattice used to obtained Λ_7^2 .

color as the central point. Thus, the theta series of Λ_7^3 begins $1 + 124q^2 + \dots$, which is an improvement over the E_7 lattice, and the next squared distance is 4.

To construct a tight packing with higher energy than E_7 in the low-density limit, we can use the hexagonal close packing in \mathbb{R}^3 , while using the same coloring on a triangular layer as for E_7 (namely, the one also used to construct E_6). The resulting coloring is shown in Fig. 3, and the packing is called Λ_7^2 . The large triangular layer at the bottom of the figure plays the same role as the central layer in the previous figures. We have not drawn the layers below it because the hcp packing is mirror symmetric about each layer.

The theta series begins $1 + 126q^2 + \dots$ for the same reason as above, but the next term is $2q^{8/3}$, which occurs between nonadjacent triangular layers. Specifically, each point in the hcp packing is at distance $\sqrt{8/3}$ (i.e., twice the height $\sqrt{2/3}$ of a regular tetrahedron with edge length 1) from two points, which are two layers above and below it. The dotted lines in Fig. 3 connect such points. Because the corresponding points always have the same color, the theta series of Λ_7^2 beings $1 + 126q^2 + 2q^{8/3} + \dots$, and hence Λ_7^2 has higher energy than E_7 in the $q \rightarrow 0$ limit.

There is one further possibility worth analyzing, namely the coloring of the hcp lattice shown in Fig. 4 which uses the Λ_6^2 coloring on a triangular layer and leads to a tight packing called Λ_7^4 . Its theta series begins $1 + 124q^2 + 2q^{8/3} + \dots$.

The four tight packings we have analyzed in this section are of course not the only tight packings, but they are the only uniform ones. Their local configurations cover enough possibilities to determine the lowest- and highest-energy tight packings. Specifically, there are relatively few period 2 colorings of a triangular layer. Observe the large triangular layers in the figures: without loss of generality we can assume that the middle horizontal row in the large triangular layer is colored $acaca$ (by the period 2 assumption), as is

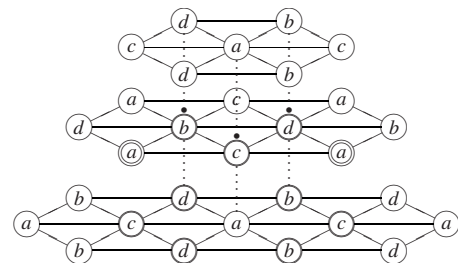


FIG. 4. The four-coloring of the hcp lattice used to obtained Λ_7^4 .

shown in each figure. Then there are only two variables in the pictures. The first is whether the adjacent two horizontal rows line up with b above b and d above d (as in Figs. 2 and 4) or whether they are staggered (as in the remaining two figures). The second variable is whether the triangular layers are themselves staggered (as in the fcc lattice) or mirror-symmetric (as in the hcp lattice). If the pictures were to be enlarged, more of these choices would arise, but within the scope of what has been drawn, there are only these four possibilities. It follows that Λ_7^3 has the best local configuration at each point, while Λ_7^2 has the worst at each point.

Theorem 5. Under postulates 2, 3, 4, and 7 of Ref. [14], the lattice Λ_7^3 has the lowest energy among all the tight seven-dimensional lattices, in the $q \rightarrow 0$ limit, and Λ_7^2 has the highest.

VIII. HIGHER DIMENSIONS

In \mathbb{R}^8 there is a unique tight packing, namely the E_8 lattice, which is almost certainly the ground state for the Gaussian core model. Because of the uniqueness of E_8 , the approach used in \mathbb{R}^5 and \mathbb{R}^7 does not apply.

Above dimension 8, the approach of Ref. [14] breaks down, and tight packings no longer fiber nicely. Outside of a handful of exceptional dimensions (certainly 24 and perhaps 12 or 16), we expect that the ground states of the Gaussian core model become quite complicated.

IX. CONCLUSIONS AND DISCUSSION

We have shown that the ground states of the Gaussian core model can be unexpectedly complex. Specifically, in five and seven dimensions, the ground states are not Bravais lattices, which contrasts with the more familiar behavior in two or three dimensions. This behavior is not limited to the Gaussian core model. The non-Bravais lattices studied in this paper are in fact superior for a wide range of soft-core models, including for example inverse power laws with high exponents. (Note that inverse power laws are scale-free, so in that case our results hold for all densities.)

These phenomena are characteristic of high dimensions, and they provide support for the Torquato-Stillinger decorrelation principle. As the dimension increases, familiar symmetries become increasingly likely to be broken. One noteworthy example is the kissing configurations in five dimensions (i.e., the spherical configurations formed by the points of tangency with adjacent spheres). The D_5 lattice's kissing configuration is highly symmetrical; in suitable coordinates it is given by the vectors $(\pm 1, \pm 1, 0, 0, 0)$ and all vectors obtained by permuting the coordinates. By contrast, the kissing configuration of Λ_5^2 is far less symmetrical. To form it, replace the eight vectors that have a 1 in the first coordinate with the eight vectors $(1, \pm 1/2, \pm 1/2, \pm 1/2, \pm 1/2)$, where the number of minus signs must be even. This clearly breaks the symmetry, and indeed the size of the symmetry group is reduced by a factor of 10 (from 3840 to 384). Nevertheless, Λ_5^2 has lower energy than D_5 , and its kissing configuration alone has lower energy than that of D_5 as spherical

configurations. Symmetry simply does not align with considerations of energy.

Because of the connections between high-dimensional sphere packing and information theory, these issues shed light on coding theory. Computer scientists and engineers have learned through long experience that efficient error-correcting codes should be chosen to be pseudo-random (truly random would be even better, but it is generally not practical). For example, MacKay (Ref. [17], p. 596) summarizes his coding theory advice as follows: "The best solution to the communication problem is: Combine a simple, pseudo-random code with a message-passing decoder." From a naive perspective, this situation is puzzling, since one might expect that highly structured codes would offer the most scope for powerful algorithms. Instead, elaborate algebraic structure seems incompatible with high-performance coding. This is not purely a geometric question, because of the role of algorithms, but it is largely geometric, and the underlying geometry involves the same decorrelation effect observed in physics. This emphasizes the need for a detailed theoretical understanding of high-dimensional packing and related statistical mechanics models.

One natural area for further exploration would be non-Euclidean spaces. Introducing curvature illuminates the problem of geometrical frustration, in which ideal local configurations do not extend consistently to global arrangements. Specifically, curvature may relieve (or introduce) frustration, and comparing results in different curvatures clarifies the role of frustration. See, for example, Ref. [18]. Much work has been done in positively curved spaces such as spheres, and Modes and Kamien [19,20] have recently studied hard-core models in negatively curved two-dimensional space. It would be intriguing to extend this work to higher dimensions.

Another area for future investigation is more sophisticated models than the Gaussian core model. For example, in the Ziherl-Kamien theory of micellar crystals [21,22], area-minimizing effects (as in soap froths) frustrate the close-packing one expects from a hard core. It would be interesting to study dimensional trends in such systems.

We conclude with a few specific open problems about the Gaussian core model.

(1) We have been able to address the low-density limit, but our approach says nothing about the high-density limit. Are Bravais lattices optimal for the Gaussian core model at high density in low dimensions, as Torquato and Stillinger [11] conjectured? We suspect that Bravais lattices may again be suboptimal in as few as five dimensions, but that is merely a guess.

(2) In this paper, we were lucky to be able to construct improved non-Bravais lattices essentially by careful modification of the Bravais lattices (much as the hcp packing can be obtained by modifying the fcc lattice). It is unlikely that this sort of modification will yield a complete picture of the Gaussian core model's ground states at all densities. In the absence of new geometrical ideas, it is natural to turn to numerical simulations. Unfortunately, simulations become increasingly difficult as the dimension increases, because of the curse of dimensionality (the number of particles required increases exponentially as a function of dimension). Can one

develop an efficient enough simulator to perform useful work in four, five, or even six dimensions? Skoge, Donev, Stillinger, and Torquato [23] have performed such simulations to compute jammed hard-core packings, but that problem may be somewhat easier as there are no long-range interactions.

(3) Is the D_4 lattice universally optimal in \mathbb{R}^4 ? (In other words, is it the ground state of the Gaussian core model at every density?) All available evidence suggests that the answer is yes, except for one observation of Cohn, Conway, Elkies, and Kumar [24]. They show that the D_4 kissing configuration of 24 points does not form a universally optimal spherical configuration, by finding a competing family of configurations that occasionally beats it. (By contrast, Cohn

and Kumar [12] proved that the E_8 kissing configuration is universally optimal.) Unfortunately, the spherical competitors do not seem to extend to Euclidean packings. Because D_4 is such a symmetrical and beautiful structure, it would be interesting to know more definitively whether it is universally optimal. Simulations could help resolve this issue.

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