ON THE HARD SPHERE MODEL AND SPHERE PACKINGS IN HIGH DIMENSIONS

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Abstract

We prove a lower bound on the *entropy* of sphere packings of $\mathbb{R}^d$ of density $\Theta(d \cdot 2^{-d})$. The entropy measures how plentiful such packings are, and our result is significantly stronger than the trivial lower bound that can be obtained from the mere existence of a dense packing. Our method also provides a new, statistical-physics-based proof of the $\Omega(d \cdot 2^{-d})$ lower bound on the maximum sphere packing density by showing that the expected packing density of a random configuration from the hard sphere model is at least $(1 + o_d(1)) \log(2/\sqrt{3})d \cdot 2^{-d}$ when the ratio of the fugacity parameter to the volume covered by a single sphere is at least $3^{-d/2}$. Such a bound on the sphere packing density was first achieved by Rogers, with subsequent improvements to the leading constant by Davenport and Rogers, Ball, Vance, and Venkatesh.

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1. Sphere packings in high dimensions

The *sphere packing density* of d-dimensional Euclidean space, $\theta(d)$, is the supremum of the packing density over all packings $\mathcal{P}$ of $\mathbb{R}^d$ by equal-sized spheres; that is,

$$\theta(d) = \sup_{\mathcal{P}} \limsup_{R \to \infty} \frac{\text{vol}(\mathcal{P} \cap B_R(0))}{\text{vol}(B_R(0))},$$

where $B_R(x)$ is the closed ball of radius R around x and $\mathrm{vol}(\mathcal{P} \cap B_R(0))$ is the volume of $B_R(0)$ covered by spheres in the packing $\mathcal{P}$. The precise value of $\theta(d)$ is known in only a small number of dimensions; to be precise for $d \in \{1, 2, 3, 8, 24\}$. While $d = 1$ is trivial and $d = 2$ is elementary but not trivial, the proof for $d = 3$ was a monumental achievement of Hales [15], and the cases $d = 8$ and $d = 24$ were proved only very recently following a breakthrough of Viazovska [37] ($d = 8$) and Cohn *et al.* [6] ($d = 24$); see [5] for an exposition of these recent developments.

Optimal sphere packings in high dimensions are even more mysterious. It is not even clear whether lattice packings achieve the optimal packing density or if the best packings are disordered. A lower bound of $\theta(d) \geqslant 2^{-d}$ is trivial. Take any saturated packing; doubling the radii of the spheres must cover all of $\mathbb{R}^d$, or else another center could be added. Therefore the original density must be at least 2^{-d}. This bound has been improved by a factor of d by Rogers [29], with subsequent improvements to the constant by Rogers and Davenport [9], Ball [2], Vance [35] (in dimensions divisible by 4), culminating in the bound of Venkatesh [36] that $\theta(d) \geqslant (65963 + o_d(1))d \cdot 2^{-d}$. Venkatesh also gains an additional $\log \log d$ factor in a sparse sequence of dimensions. An upper bound of $\theta(d) \leqslant 2^{-(.599\cdots + o_d(1)) \cdot d}$ is due to Kabatiansky and Levenshtein [20]; Cohn and Zhao [7] made a recent constant factor improvement. Here we write $h(d) = o_d(1)$ if $h(d) \to 0$ as $d \to \infty$. We write $h_1(d) = \Omega(h_2(d))$ if $h_1(d)/h_2(d) \geqslant c > 0$ for all sufficiently large d and some constant c, and $h_1(d) = \Theta(h_2(d))$ if $0 < c \leqslant h_1(d)/h_2(d) \leqslant C$ for all sufficiently large d and two constants c, C. We caution the reader to distinguish between the similar characters $\theta(d)$ and $\Theta(\cdot)$.

Notably there has been no progress in closing the gap on an exponential scale between the trivial lower bound and the Kabatiansky and Levenshtein upper bound. See the books of Rogers [30], Conway and Sloane [8], and Cohn [4] for an overview of results and techniques in the area.

Several of the previous proofs of lower bounds on $\theta(d)$ analyze a random lattice packing by way of the Siegel mean-value theorem [33] or variants thereof; a bound of $2 \cdot 2^{-d}$ is achieved by analyzing a uniform random lattice (see [4, Proposition 6.1]); by imposing additional symmetries on the random lattice Vance [35] and Venkatesh [36] gain a factor d and an improved constant. But optimal packings in high dimensions are not necessarily lattice packings (see the conjectures of Torquato and Stillinger [34]). If this is so, then we need different tools and constructions. One natural candidate is the *hard sphere model* from statistical physics ('hard' spheres since the only interaction between particles is the hard constraint that spheres cannot overlap). This is a probability distribution over sphere packings governed by a fugacity parameter $\lambda > 0$. The larger λ, the larger the typical density of a random packing from the model.

Here we utilize the hard sphere model to analyze sphere packings in high dimensions. We show that for an appropriate choice of the fugacity, the expected packing density of a configuration drawn from the hard sphere model is $\Omega(d \cdot 2^{-d})$. The argument not only gives a statistical physics proof of the lower bound on $\theta(d)$, but also gives a lower bound on the entropy of sphere packings of this density. We define the entropy precisely in Section 2, but it essentially expresses the exponential order of the fraction of sets of αn points in a ball of volume n that are centers of a valid sphere packing in $\mathbb{R}^d$. That is, it is a measure of how plentiful packings of a given density are.

The proof technique is general; in fact a version of the argument in a discrete setting [11] (where the relevant statistical physics model is the hard-core model) states that a uniformly random independent set chosen from a triangle-free graph of maximum degree r occupies at least a $\log r / r$ fraction of the vertices in expectation. This result gives an alternative proof of Shearer's bound of Ramsey number $R(3, k) \leqslant (1 + o(1))k^2 / \log k$ [32], which is itself a sharpening of the independent set result of Ajtai *et al.* [1] used by Krivelevich *et al.* [22] (following [19]) to give an alternative proof of the $\Omega(d \cdot 2^{-d})$ lower bound on $\theta(d)$ by formulating the problem in terms of finding a large independent set in a graph derived by discretizing a region in $\mathbb{R}^d$. Since the first version of this paper, we have also used a variant of the method to prove lower bounds on the kissing number and size of spherical codes in high dimensions [18].

In principle, the hard sphere model is a good random model with which to study optimal and near optimal sphere packings, as typical packings from the model will have density arbitrarily close to $\theta(d)$ for a large enough choice of the fugacity parameter λ. Analyzing the typical packing density, however, is another matter, and we do not expect our particular technique, which relies only on local information, to improve the exponential order of the lower bound on $\theta(d)$. In the analogy with independent sets in graphs, the $\Omega(d \cdot 2^{-d})$ bound corresponds to the $\Omega(\log r / r)$ lower bound on the independence ratio of a r-regular triangle-free graph. However, random r-regular graphs and random r-regular bipartite graphs have the same local structure asymptotically yet have drastically different independence ratios: $2 \log r / r$ and $1/2$, respectively.

In Section 2, we explain the hard sphere model in detail and state our main result (Theorem 2). In Section 3, we prove Theorem 2. In Section 4, we use Theorem 2 to prove a lower bound on the volume of sphere packings of density $\Theta(d \cdot 2^{-d})$. This lower bound is significantly larger than the trivial bound obtained by shrinking the spheres of a dense packing and allowing the centers to move locally.

In what follows $\log x$ always denotes the natural logarithm of x. For $x, y \in \mathbb{R}^d$, we let $d(x, y)$ denote the Euclidean distance between x and y, and for $X \subseteq \mathbb{R}^d$

we let $d(X, y) = \inf_{x \in X} d(x, y)$. The sphere of radius r centered at x in $\mathbb{R}^d$ is $\{y : d(x, y) = r\}$, while the (open) ball of radius r is $\{y : d(x, y) < r\}$.

2. The hard sphere model

The *hard sphere model* is a probability distribution over configurations of nonoverlapping, identical spheres in a bounded subset of Euclidean space (that can be extended with a limiting argument to a distribution on packings of all of $\mathbb{R}^d$). There are two variants of the model: the *canonical ensemble* is a uniformly random packing of a given fixed density and the *grand canonical ensemble* is a random packing with variable density governed by a fugacity parameter $\lambda > 0$. The hard sphere model is a simple model of a gas or fluid with no interactions apart from the hard constraint that molecules cannot overlap. In dimension 2 and 3 the model is expected to exhibit a *freezing* phase transition, though proving this remains an open mathematical problem. Such a phase transition would show that freezing and crystallization can be explained by purely geometric concerns. The nature of such a phase transition may be different in 2 dimensions than in 3: Richthammer [28] has proved that there can be no translational symmetry breaking in dimension 2. For more see Löwen's survey [23].

To define the model precisely, we assume the spheres of our packings have volume 1 and denote by r_d the radius of a ball of volume 1 in $\mathbb{R}^d$. For a bounded, measurable subset $S \subset \mathbb{R}^d$, let $C_k(S)$ be the set of unordered k-tuples of points from S; that is,

$$C_k(S) = \{\{x_1, \ldots x_k\} : x_i \in S \,\forall i\}.$$

Let

$$P_k(S) = \{\{x_1, \ldots x_k\} \in C_k(S) : d(x_i, x_j) > 2r_d \,\forall i \neq j\};$$

that is, $P_k(S)$ is the subset of $C_k(S)$ consisting of the centers of packings of spheres of volume 1. Note that we allow centers near the boundary of S, so the spheres themselves need not lie entirely within S.

The *canonical hard sphere model* on S with k centers is simply a uniformly random k-tuple $\mathbf{X}_k \in P_k(S)$. The *partition function* of the canonical hard sphere model on S is the function

$$\hat{Z}_S(k) = \frac{1}{k!} \int_{S^k} \mathbf{1}_{\mathcal{D}(x_1, \ldots, x_k)} \, dx_1 \cdots dx_k, \tag{1}$$

where for $x_1, \ldots, x_k \in \mathbb{R}^d$, the expression $\mathcal{D}(x_1, \ldots, x_k)$ denotes the event that $d(x_i, x_j) > 2r_d$ for all distinct $i, j \in [k]$. In other words, $\hat{Z}_k(S)$ is the volume of $P_k(S)$ in the space of unordered k-tuples from S. As the volume of $C_k(S)$

is $\mathrm{vol}(S)^k/k!$, the probability that k uniformly random points in S are the centers of a sphere packing is $(k!/\mathrm{vol}(S)^k)\hat{Z}_S(k)$.

In the canonical ensemble the number of centers is fixed. In the grand canonical ensemble we imagine S lying in some larger region with which it can exchange particles, and so the number of centers is allowed to fluctuate.

The *grand canonical hard sphere model* on a bounded, measurable set $S \subset \mathbb{R}^d$ at fugacity λ is a random set $\mathbf{X}$ of unordered points, with $\mathbf{X}$ distributed according to a Poisson point process of intensity λ conditioned on the event that $d(x, y) > 2r_d$ for all distinct $x, y \in \mathbf{X}$.

The partition function of the grand canonical hard sphere model on S is

$$Z_S(\lambda) = \sum_{k \geqslant 0} \lambda^k \hat{Z}_S(k) \qquad (2)$$

where we take $\hat{Z}_S(0) = 1$. If S is bounded then $Z_S(\lambda)$ is a polynomial in λ.

Note that the fugacity λ is not an absolute quantity: defining the model with spheres of a different size would lead to a different scaling of the fugacity. The right absolute parameter to consider is the ratio of the fugacity to the volume enclosed by a single hard sphere; as we consider spheres of volume 1 here, this ratio is λ as well.

In both the canonical and grand canonical ensembles, the partition function and its normalized logarithm play a central role in the study of the hard sphere model. Let $B_n = B_{n^{1/d} \cdot r_d}(0)$ be the ball of volume n around the origin in $\mathbb{R}^d$. The limits

$$f_d(\alpha) := \lim_{n \to \infty} \frac{1}{\alpha n} \log \frac{\hat{Z}_{B_n}(\lfloor \alpha n \rfloor)}{n^{\lfloor \alpha n \rfloor}/(\lfloor \alpha n \rfloor)!}$$

$$g_d(\lambda) := \lim_{n \to \infty} \frac{1}{n} \log Z_{B_n}(\lambda)$$

exist for $\alpha \in (0, \theta(d))$ and $\lambda > 0$ (see for example [31, Ch. 3]). We will call $f_d(\alpha)$ the *entropy density* of sphere packings of $\mathbb{R}^d$ at density α, and $g_d(\lambda)$ the *pressure* of the hard sphere model. Both are measurements of how plentiful sphere packings are in $\mathbb{R}^d$. The entropy density is minus the thermodynamic *free energy*, which itself is the large deviation rate function of the probability that αn random points in B_n form a sphere packing. We dispense with the minus sign so that a lower bound on $f_d(\alpha)$ corresponds to a lower bound on the quantity of sphere packings. Dividing by αn ensures that $f_d(\alpha)$ is independent of the choice of the size of spheres in our packings. See for example [27] for a discussion of the entropy density in dimension 3.

The statistical physics definition of a phase transition in the hard sphere model is that the entropy density (respectively the pressure) is nonanalytic at some

$\alpha^* \in (0, \theta(d))$ (respectively at some $\lambda^* > 0$). See [13, 17, 26] for some recent results showing that the entropy density or pressure is analytic below some threshold in α or λ. See also [12, 16, 21] for results showing that certain Markov chains for sampling from these models mix rapidly below a given threshold.

In fact in the large volume limit the two ensembles are essentially equivalent, as for each $\lambda > 0$, there is a typical density $\alpha(d, \lambda)$ with small fluctuations. However, computing this conversion function $\alpha(d, \lambda)$ is as difficult as understanding both the sphere packing problem and the problem of phase transitions in the hard sphere model, as $\lim_{\lambda \to \infty} \alpha(d, \lambda) = \theta(d)$ (for example [24]) and $\alpha(d, \lambda)$ is nonanalytic at λ at which $g_d(\lambda)$ is nonanalytic. The main task of this work is to prove a lower bound on $\alpha(d, \lambda)$.

The *expected packing density*, $\alpha_S(\lambda)$, of the hard sphere model is simply the expected number of centers in S normalized by the volume of S; that is,

$$\alpha_S(\lambda) = \frac{\mathbb{E}_{S,\lambda}|\mathbf{X}|}{\text{vol}(S)}.$$

Here and in what follows the notation $\mathbb{P}_{S,\lambda}$ and $\mathbb{E}_{S,\lambda}$ indicates probabilities and expectations with respect to the grand canonical hard sphere model on a region S at fugacity λ. We may omit the subscripts if S and λ are clear from the context.

The expected packing density can be expressed as the derivative of the normalized log partition function. We calculate

$$\alpha_S(\lambda) = \frac{1}{\text{vol}(S)} \sum_{k=1}^{\infty} k \cdot \mathbb{P}_{S,\lambda}[|\mathbf{X}| = k]$$

$$= \frac{1}{\text{vol}(S)} \sum_{k=1}^{\infty} \frac{k \cdot \lambda^k \hat{Z}_S(k)}{Z_S(\lambda)}$$

$$= \frac{1}{\text{vol}(S)} \frac{\lambda \cdot Z_S'(\lambda)}{Z_S(\lambda)} \tag{3}$$

$$= \frac{\lambda}{\text{vol}(S)} (\log Z_S(\lambda))'. \tag{4}$$

The next lemma shows that the expected packing density of the hard sphere model provides a lower bound for $\theta(d)$.

LEMMA 1. *The asymptotic expected packing density of $B_n \subset \mathbb{R}^d$ is a lower bound on the maximum sphere packing density. That is, for any $\lambda > 0$,*

$$\theta(d) \geqslant \limsup_{n \to \infty} \alpha_{B_n}(\lambda).$$

Proof. First note that

$$\theta(d) = \limsup_{n \to \infty} \sup_{X \in \mathcal{P}(B_n, r_d)} \frac{|X|}{n} \qquad (5)$$

where $\mathcal{P}(B_n, r_d)$ is the set of all packings of B_n by spheres of radius r_d (where again only the centers need to be in B_n); that is, sets of distinct points $X \subset B_n$ so that $d(x_i, x_j) > 2r_d$ for all distinct $x_i, x_j \in X$. The equality (5) relies on the fact that volume of a ball in $\mathbb{R}^d$ grows subexponentially fast as a function of its radius, and so deleting centers from the boundary of B_n has a negligible effect on the packing density as $n \to \infty$. Now from the definition of the expected packing density, $\sup_{X \in \mathcal{P}(B_n, r_d)} (|X|/n) \geqslant \alpha_{B_n}(\lambda)$ for any λ.   □

Our main result is the following lower bound on the expected packing density.

THEOREM 2. *Let $S \subset \mathbb{R}^d$ be bounded, measurable, and of positive volume. Then for any $\lambda \geqslant 3^{-d/2}$, we have*

$$\alpha_S(\lambda) \geqslant (1 + o_d(1)) \frac{\log(2/\sqrt{3}) \cdot d}{2^d}.$$

We remark that the error term in Theorem 2 can be taken to be $O(\log d / d)$ uniformly over the choice of λ and S. As a corollary, by applying Theorem 2 to B_n, we obtain the following lower bound on the sphere packing density of the d-dimensional Euclidean space.

COROLLARY 3.

$$\theta(d) \geqslant (1 + o_d(1)) \frac{\log(2/\sqrt{3}) \cdot d}{2^d}.$$

The fact that we achieve the bound in Theorem 2 for λ as small as $3^{-d/2}$ has no implication on the bound obtained on $\theta(d)$, but it allows us to prove nontrivial lower bounds on the entropy density and pressure.

THEOREM 4. *For all $\lambda = e^{-cd}$ with $c \in [(\log 3)/2, \log 2)$,*

$$g_d(\lambda) \geqslant \left(\frac{(\log 2 - c)^2}{2} + o_d(1) \right) \cdot \frac{d^2}{2^d}.$$

THEOREM 5. *There exists $\alpha = \alpha(d) = (1 + o_d(1))((\log(2/\sqrt{3}) \cdot d)/2^d)$ so that*

$$f_d(\alpha) \geqslant -(1 + o_d(1)) \log(2/\sqrt{3}) \cdot d.$$

The lower bound in Theorem 5 matches, up to a factor 2, a formula for the entropy of hard spheres conjectured in the physics literature to hold for densities

up to either the crystallization phase transition or the glass transition, whichever comes first [**14**, **25**] (see also [**3**] for an overview of the mean-field approach to hard spheres).

Of course even the existence of a sphere packing of density $\Theta(d \cdot 2^{-d})$ implies some positive volume of sphere packings at a slightly lower density by shrinking the spheres and allowing their centers to move locally. Such a lower bound on the canonical partition function is called the 'cell model' lower bound in statistical physics (see for example [**23**, Section 4.2]). While the cell model is a rigorous lower bound on $\hat{Z}_S(k)$ at all densities, it is thought to be approximately accurate if the model is in a crystalline phase. In Section 4.1 we compare the bound from Theorem 5 to this cell model lower bound, and show that it is significantly stronger.

In fact, to achieve the bound in Theorem 5 through the existence of a dense packing and the cell model lower bound would require $\theta(d) \geqslant (2 - \varepsilon)^{-d}$ for some $\varepsilon > 0$. So in a sense we can say that either there is no crystallization at density $\Theta(d \cdot 2^{-d})$ or there are exponentially better sphere packings than currently known. We leave precise statements to this effect for future work, but conclude by observing that these two challenging problems in geometry and statistical physics, determining the asymptotic sphere packing density and determining whether or not the hard sphere model exhibits a phase transition, closely complement one another and understanding their relationship may open the way to further progress in both areas.

3. A lower bound on the expected packing density

In this section we prove Theorem 2. We start with some useful identities and inequalities.

When λ is large, the model favors configurations with more spheres. It is a standard fact that $\alpha_S(\lambda)$ is strictly increasing in λ.

LEMMA 6. *Let $S \subset \mathbb{R}^d$ be bounded, measurable, and of positive volume. Then the expected packing density $\alpha_S(\lambda)$ is a strictly increasing function of λ.*

Proof. We use (4) and calculate

$$
\lambda \cdot \text{vol}(S) \cdot \alpha'_S(\lambda) = \lambda^2 (\log Z_S(\lambda))'' + \lambda (\log Z_S(\lambda))'
$$

$$
= \lambda^2 \cdot \frac{Z_S(\lambda) Z''_S(\lambda) - (Z'_S(\lambda))^2}{Z_S^2(\lambda)} + \frac{\lambda Z'_S(\lambda)}{Z_S(\lambda)}
$$

$$
= \mathbb{E}_{S,\lambda}[|\mathbf{X}|(|\mathbf{X}| - 1)] - (\mathbb{E}_{S,\lambda}[|\mathbf{X}|])^2 + \mathbb{E}_{S,\lambda}[|\mathbf{X}|]
$$

$$
= \text{var}_{S,\lambda}[|\mathbf{X}|] > 0,
$$

and so $\alpha_S(\lambda)$ is strictly increasing. □

Let $\mathrm{FV}_S(\lambda)$ denote the expected *free volume* of the hard sphere model; that is, the expected fraction of the volume of S containing points that are at distance at least $2r_d$ from the nearest center; or in other words, the expected fraction of volume at which a new sphere could be legally placed. A key fact in our argument is the following link between $\alpha_S(\lambda)$ and $\mathrm{FV}_S(\lambda)$.

LEMMA 7. *Let $S \subset \mathbb{R}^d$ be bounded, measurable, and of positive volume. Then*

$$\alpha_S(\lambda) = \lambda \cdot \mathrm{FV}_S(\lambda).$$

Proof. We simply use the definition of $\alpha_S(\lambda)$ and compute

$$
\begin{aligned}
\alpha_S(\lambda) &= \frac{\mathbb{E}_{S,\lambda}|\mathbf{X}|}{\mathrm{vol}(S)} \\
&= \frac{1}{\mathrm{vol}(S)} \sum_{k=0}^{\infty} (k+1)\mathbb{P}_{S,\lambda}[|\mathbf{X}| = k+1] \\
&= \frac{1}{\mathrm{vol}(S)Z_S(\lambda)} \sum_{k=0}^{\infty} \int_{S^{k+1}} \frac{\lambda^{k+1}}{k!} \mathbf{1}_{\mathcal{D}(x_0,\ldots,x_k)} \, dx_1 \cdots dx_k dx_0 \\
&= \frac{\lambda}{\mathrm{vol}(S)Z_S(\lambda)} \int_S \left[1 + \sum_{k=1}^{\infty} \int_{S^k} \frac{\lambda^k}{k!} \mathbf{1}_{\mathcal{D}(x_0,\ldots,x_k)} \, dx_1 \cdots dx_k \right] dx_0 \\
&= \lambda \cdot \mathrm{FV}_S(\lambda). \qquad \square
\end{aligned}
$$

Now consider the following two-part experiment: sample a configuration of centers $\mathbf{X}$ from the hard sphere model on S at fugacity λ and independently choose a point $\mathbf{v}$ uniformly from S. We define the random set

$$\mathbf{T} = \{x \in B_{2r_d}(\mathbf{v}) \cap S : d(x, y) > 2r_d \,\, \forall \, y \in \mathbf{X} \cap B_{2r_d}(\mathbf{v})^c\}.$$

That is, $\mathbf{T}$ is the set of all points of S in the $2r_d$ ball around $\mathbf{v}$ that are not blocked from being a center by a center outside the $2r_d$ ball around $\mathbf{v}$. We call $\mathbf{T}$ the set of externally uncovered points in the neighborhood of $\mathbf{v}$, in analogy with the terminology used in [10, 11] in the discrete case. Note that $\mathbf{T}$ depends only on $\mathbf{X} \cap B_{2r_d}(\mathbf{v})^c$—the presence or absence of centers inside $B_{2r_d}(\mathbf{v})$ has no effect on $\mathbf{T}$ (see Figure 1).

Since $\mathbf{X}$ is a finite set of points it is clear that there exists some $\varepsilon > 0$ (depending on $\mathbf{X}$) such that $B_\varepsilon(\mathbf{v}) \cap S \subseteq \mathbf{T}$. If S has positive volume then it follows from the Lebesgue density theorem that $B_\varepsilon(\mathbf{v}) \cap S$ has positive volume almost surely and hence that $\mathrm{vol}(\mathbf{T}) > 0$ almost surely.
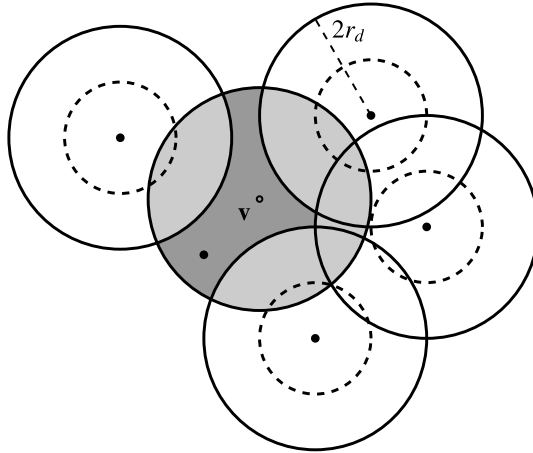
Figure 1. An illustration of the set of externally uncovered points in the neighborhood of **v** (shaded dark gray). The dashed circles represent the hard spheres which do not overlap.

PROPOSITION 8. *Let $S \subset \mathbb{R}^d$ be bounded, measurable, and of positive volume. Then*

$$\alpha_S(\lambda) = \lambda \cdot \mathbb{E}\left[\frac{1}{Z_{\mathbf{T}}(\lambda)}\right] \tag{6}$$

and

$$\alpha_S(\lambda) \geqslant 2^{-d} \cdot \mathbb{E}\left[\frac{\lambda \cdot Z'_{\mathbf{T}}(\lambda)}{Z_{\mathbf{T}}(\lambda)}\right], \tag{7}$$

where both expectations are with respect to the random set $\mathbf{T}$ generated by the two-part experiment defined above.

Proof. We use Lemma 7 to conclude that

$$\begin{aligned}
\alpha_S(\lambda) &= \lambda \cdot \mathrm{FV}_S(\lambda) \\
&= \frac{\lambda}{\mathrm{vol}(S)} \int_S \mathbb{P}[d(\mathbf{X}, v) > 2r_d] \, dv \\
&= \lambda \cdot \mathbb{E}[\mathbf{1}_{\mathbf{T} \cap \mathbf{X} = \emptyset}] \\
&= \lambda \cdot \mathbb{E}\left[\frac{1}{Z_{\mathbf{T}}(\lambda)}\right],
\end{aligned}$$

which gives (6). The last equality uses the spatial Markov property of the hard sphere model: conditioned on $\mathbf{X} \cap B_{2r_d}(\mathbf{v})^c$, the distribution of $\mathbf{X} \cap B_{2r_d}(\mathbf{v})$ is exactly that of the hard sphere model on the set $\mathbf{T}$.

Now, for any $x \in S$, $\mathbb{P}(x \in B_{2r_d}(\mathbf{v})) = \mathrm{vol}(S \cap B_{2r_d}(x))/\mathrm{vol}(S) \leqslant 2^d/\mathrm{vol}(S)$. It follows that

$$
\begin{aligned}
\alpha_S(\lambda) &\geqslant 2^{-d} \cdot \mathbb{E}[|\mathbf{X} \cap B_{2r_d}(\mathbf{v})|] \\
&= 2^{-d} \cdot \mathbb{E}[\alpha_{\mathbf{T}}(\lambda) \cdot \mathrm{vol}(\mathbf{T})] \\
&\overset{(3)}{=} 2^{-d} \cdot \mathbb{E}\left[\frac{\lambda \cdot Z'_{\mathbf{T}}(\lambda)}{Z_{\mathbf{T}}(\lambda)} \right]. \qquad \square
\end{aligned}
$$

PROPOSITION 9. *Let $S \subset \mathbb{R}^d$ be bounded and measurable. Then*

$$
\log Z_S(\lambda) \leqslant \lambda \cdot vol(S) \tag{8}
$$

and if in addition S is of positive volume, then

$$
\alpha_S(\lambda) \geqslant \lambda \cdot e^{-\lambda \cdot \mathbb{E}[vol(\mathbf{T})]}. \tag{9}
$$

Proof. From (2), the definition of $Z_S(\lambda)$, we have $Z_S(\lambda) \leqslant \sum_{k=0}^{\infty} (\lambda^k/k!) \cdot \mathrm{vol}(S)^k = e^{\lambda \cdot \mathrm{vol}(S)}$. Turning to (9), we conclude

$$
\begin{aligned}
\alpha_S(\lambda) &\overset{(6)}{=} \lambda \cdot \mathbb{E}\left[\frac{1}{Z_{\mathbf{T}}(\lambda)} \right] \\
&\overset{(8)}{\geqslant} \lambda \cdot \mathbb{E}[e^{-\lambda \cdot \mathrm{vol}(\mathbf{T})}] \\
&\geqslant \lambda \cdot e^{-\lambda \cdot \mathbb{E}[\mathrm{vol}(\mathbf{T})]},
\end{aligned}
$$

where the last inequality is an application of Jensen's Inequality. $\square$

LEMMA 10. *Let $S \subseteq B_{2r_d}(0)$ be measurable. Then*

$$
\mathbb{E}[vol(B_{2r_d}(\mathbf{u}) \cap S)] \leqslant 2 \cdot 3^{d/2}, \tag{10}
$$

where $\mathbf{u}$ is a uniformly chosen point in S. In particular

$$
\alpha_S(\lambda) \geqslant \lambda \cdot e^{-\lambda \cdot 2 \cdot 3^{d/2}}. \tag{11}
$$

The geometric fact (10) is related to the fact used in [22]; here we consider the volume of the intersection of a sphere with an arbitrary set, but we bound this by the intersecting volume of two identical spheres, as in [22].
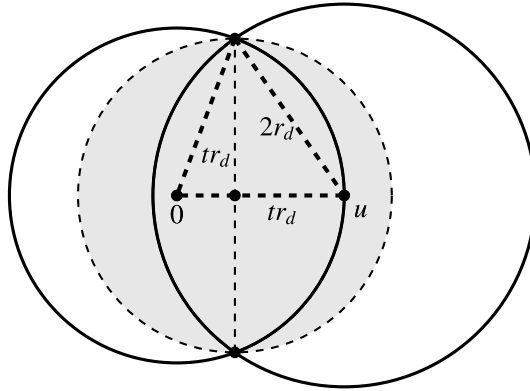
Figure 2. We upper bound the volume of the intersection of two spheres, centered at 0 and u, with radii tr_d and $2r_d$ respectively, by the volume of the smallest sphere, depicted in gray, containing the intersection.

Proof of Lemma 10. Clearly, we may assume that S has positive volume. We write

$$\mathbb{E}[\text{vol}(B_{2r_d}(\mathbf{u}) \cap S)] = \frac{1}{\text{vol}(S)} \int_S \int_S \mathbf{1}_{d(u,v) \leqslant 2r_d} \, dv \, du$$

$$= \frac{2}{\text{vol}(S)} \int_S \int_S \mathbf{1}_{d(u,v) \leqslant 2r_d} \cdot \mathbf{1}_{\|v\| \leqslant \|u\|} \, dv \, du$$

$$\leqslant 2 \max_{u \in B_{2r_d}(0)} \int_S \mathbf{1}_{d(u,v) \leqslant 2r_d} \cdot \mathbf{1}_{\|v\| \leqslant \|u\|} \, dv$$

$$\leqslant 2 \max_{u \in B_{2r_d}(0)} \text{vol}(B_{2r_d}(u) \cap B_{\|u\|}(0)).$$

Now suppose the point u is at distance tr_d from 0 for some $t \in [0, 2]$. We may assume that $t \geqslant \sqrt{2}$ as otherwise $\text{vol}(B_{\|u\|}(0)) \leqslant 2^{d/2}$. Then, by bounding the volume of the intersection of two balls by the volume of a containing ball (see Figure 2), we have

$$\text{vol}(B_{2r_d}(u) \cap B_{tr_d}(0)) \leqslant \text{vol}(B_{2r_d\sqrt{1-t^{-2}}}(0))$$

$$\leqslant \left(2\sqrt{1-t^{-2}}\right)^d,$$

and so

$$\mathbb{E}[\text{vol}(B_{2r_d}(\mathbf{u}) \cap S)] \leqslant \max\left\{2^{d/2}, 2 \cdot \max_{\sqrt{2} \leqslant t \leqslant 2} \left(2\sqrt{1-t^{-2}}\right)^d\right\}$$

$$= 2 \cdot 3^{d/2}.$$

This establishes (10). It follows that $\mathbb{E}[\text{vol}(\mathbf{T})] \leqslant 2 \cdot 3^{d/2}$ and so (11) follows from (9). □

Using these results we now prove Theorem 2.

Proof of Theorem 2. Let $S \subset \mathbb{R}^d$ be bounded, measurable, and of positive volume. Let $\alpha = \alpha_S(\lambda)$. Then by Jensen's Inequality we obtain

$$\alpha \overset{(6)}{=} \lambda \cdot \mathbb{E}\left[\frac{1}{Z_{\mathbf{T}}(\lambda)}\right] \geqslant \lambda \cdot e^{-\mathbb{E}\log Z_{\mathbf{T}}(\lambda)},$$

where as above the expectation is with respect to the two-part experiment in forming the random set $\mathbf{T}$.

On the other hand we have

$$\begin{aligned}
\alpha &\overset{(7)}{\geqslant} 2^{-d} \cdot \mathbb{E}\left[\frac{\lambda \cdot Z'_{\mathbf{T}}(\lambda)}{Z_{\mathbf{T}}(\lambda)}\right] \\
&\overset{(3)}{=} 2^{-d} \cdot \mathbb{E}[\text{vol}(\mathbf{T}) \cdot \alpha_{\mathbf{T}}(\lambda)] \\
&\overset{(11)}{\geqslant} 2^{-d} \cdot \mathbb{E}[\lambda \cdot \text{vol}(\mathbf{T}) \cdot e^{-\lambda \cdot 2 \cdot 3^{d/2}}] \\
&\overset{(8)}{\geqslant} 2^{-d} \cdot \mathbb{E}[\log Z_{\mathbf{T}}(\lambda) \cdot e^{-\lambda \cdot 2 \cdot 3^{d/2}}] \\
&= 2^{-d} \cdot e^{-\lambda \cdot 2 \cdot 3^{d/2}} \mathbb{E}[\log Z_{\mathbf{T}}(\lambda)].
\end{aligned}$$

Combining these two lower bounds, and letting $z = \mathbb{E}\log Z_{\mathbf{T}}(\lambda)$, we see that

$$\alpha \geqslant \inf_z \max\{\lambda e^{-z}, z \cdot 2^{-d} e^{-\lambda \cdot 2 \cdot 3^{d/2}}\}.$$

Since λe^{-z} is decreasing in z and $z \cdot 2^{-d} e^{-\lambda \cdot 2 \cdot 3^{d/2}}$ increasing, the infimum over z of the maximum of the two expressions occurs when they are equal, that is, $\alpha \geqslant \lambda e^{-z^*}$, where z^* is the solution to

$$\lambda e^{-z} = z \cdot 2^{-d} e^{-\lambda \cdot 2 \cdot 3^{d/2}},$$

or in other words,

$$z^* = W(\lambda 2^d e^{\lambda \cdot 2 \cdot 3^{d/2}}) \tag{12}$$

where $W(\cdot)$ is the Lambert-W function. For readers unfamiliar with the W function we take a moment to recall some of its properties. For $x > 0$, $w = W(x)$ is defined to be the unique solution to the equation $we^w = x$. Taking logarithms yields $w + \log w = \log x$ and so

$$w = \log x - \log(\log x - \log w) = \log x - \log \log x - \log\left(1 - \frac{\log w}{\log x}\right).$$

It follows that as $x \to \infty$,

$$W(x) = \log x - \log \log x + O\left(\frac{\log \log x}{\log x}\right). \tag{13}$$

Now, returning to (12), we take $\lambda = d^{-1}3^{-d/2}$ (in fact $\lambda = \varepsilon 3^{-d/2}$ for any $\varepsilon = \varepsilon(d)$ such that $\varepsilon \to 0$ and $-\log(\varepsilon)/d \to 0$ as $d \to \infty$ would suffice). Using (13), this gives

$$\begin{aligned} z^* &= W(\lambda \cdot 2^d \cdot e^{2/d}) \\ &= \log \lambda + d \log 2 - \log d - \log \log(2/\sqrt{3}) + O(\log d/d) \end{aligned}$$

and so

$$\alpha \geqslant \lambda e^{-z^*} = \left(1 + O\left(\frac{\log d}{d}\right)\right) \frac{\log(2/\sqrt{3}) \cdot d}{2^d}.$$

Recalling that α is monotone in λ (Lemma 6), this bound holds for all $\lambda \geqslant d^{-1}3^{-d/2}$. This completes the proof of Theorem 2. $\qquad\square$

Note that in the proof if we take $\lambda = e^{-cd}$ for $c \in ((\log 3)/2, \log 2)$, then we obtain the following bound

$$\alpha_S(\lambda) \geqslant (1 + o_d(1)) \frac{(\log 2 - c) \cdot d}{2^d}. \tag{14}$$

4. A lower bound on the entropy density and pressure

We first consider the grand canonical model and the pressure of the hard sphere model. As shown in (4), the expected packing density is the scaled derivative of the log partition function; that is $\alpha_S(\lambda) = (\lambda/\mathrm{vol}(S))(\log Z_S(\lambda))'$. Theorem 2 and inequality (14) give a lower bound on the expected packing density; by integrating this bound we obtain the lower bound on the pressure stated in Theorem 4.

Proof of Theorem 4. We compute

$$\begin{aligned} \frac{1}{n} \log Z_{B_n}(\lambda) &= \int_0^\lambda \frac{1}{n} (\log Z_{B_n}(t))' \, dt \\ &= \int_0^\lambda \frac{\alpha_{B_n}(t)}{t} \, dt \end{aligned}$$

$$\geqslant -d \int_{\log 2}^{c} \alpha_{B_n}(e^{-ud}) \, du$$

$$\geqslant (1 + o_d(1)) \frac{d^2}{2^d} \int_{c}^{\log 2} (\log 2 - u) \, du$$

$$= \left(\frac{(\log 2 - c)^2}{2} + o_d(1) \right) \cdot \frac{d^2}{2^d},$$

and taking $n \to \infty$ gives the theorem. $\qquad\square$

Now recall the definition of the entropy density of sphere packings of $\mathbb{R}^d$ at density α:

$$f_d(\alpha) = \lim_{n \to \infty} \frac{1}{\alpha n} \log \frac{\hat{Z}_{B_n}(\lfloor \alpha n \rfloor)}{n^{\lfloor \alpha n \rfloor} / (\lfloor \alpha n \rfloor)!}.$$

The entropy density is a measure of how plentiful sphere packings of a given density are, as it tells us, on a logarithmic scale, what fraction of point sets of a given density in a large region of $\mathbb{R}^d$ are the centers of a sphere packing. We use Theorem 2 to provide the lower bound on $f_d(\alpha)$ given in Theorem 5. First let us record the simple fact that as sphere packings become more dense they become less plentiful.

LEMMA 11. *$f_d(\alpha)$ is decreasing in α.*

Proof. Suppose $0 < \alpha < \alpha' < \theta(d)$. Since the limit

$$f_d(\alpha) = \lim_{n \to \infty} \frac{1}{\alpha n} \log \frac{\hat{Z}_{B_n}(\lfloor \alpha n \rfloor)}{n^{\lfloor \alpha n \rfloor} / (\lfloor \alpha n \rfloor)!}$$

exists it is enough to show

$$\frac{1}{\alpha n} \log \frac{\hat{Z}_{B_n}(\lfloor \alpha n \rfloor)}{n^{\lfloor \alpha n \rfloor} / (\lfloor \alpha n \rfloor)!} \geqslant \frac{1}{\alpha' n'} \log \frac{\hat{Z}_{B_{n'}}(\lfloor \alpha' n' \rfloor)}{n'^{\lfloor \alpha' n' \rfloor} / (\lfloor \alpha' n' \rfloor)!}$$

for some sequence $n, n' \to \infty$. Choose n arbitrarily and set $n' = (\alpha / \alpha')n$. Let $k_0 = \alpha n = \alpha' n'$ and $k = \lfloor \alpha n \rfloor = \lfloor \alpha' n' \rfloor$. Then we must show

$$\frac{1}{k_0} \log \frac{\hat{Z}_{B_n}(k)}{n^k / k!} \geqslant \frac{1}{k_0} \log \frac{\hat{Z}_{B_{n'}}(k)}{n'^k / k!},$$

or equivalently,

$$\frac{\hat{Z}_{B_n}(k)}{n^k} \geqslant \frac{\hat{Z}_{B_{n'}}(k)}{n'^k}.$$

In words this is the statement that the probability k uniform and independent random points in a ball of volume n form a packing of balls of volume 1 is at least the same probability in a ball of volume n' with $n' < n$. This follows from a simple scaling and coupling: it is the same as the statement that the probability k uniform and independent random points in a ball of volume n form a packing of balls of volume 1 is at least the probability k uniform and independent random points in a ball of volume n form a packing of balls of volume v with $v > 1$, and clearly the second event is contained in the first.   □

Now we prove our lower bound on the entropy density.

Proof of Theorem 5. In the following there is a lot of flexibility in our choice of parameters and we do not attempt to optimize all of our bounds. Fix d and n sufficiently large. Choose $\lambda \in [3^{-d/2}, 2 \cdot 3^{-d/2}]$ so that $\mathrm{var}_{B_n,\lambda}|\mathbf{X}| \leqslant n^{3/2}$; such a choice of λ always exists because otherwise, by the calculation of Lemma 6, we would have

$$\alpha_{B_n}(2 \cdot 3^{-d/2}) = \frac{1}{n} \int_0^{2 \cdot 3^{-d/2}} \frac{\mathrm{var}_{B_n,t}|\mathbf{X}|}{t} \, dt \geqslant \frac{1}{n} \int_{3^{-d/2}}^{2 \cdot 3^{-d/2}} \frac{n^{3/2}}{t} \, dt = n^{1/2} \cdot \log 2 > 1.$$

By our bound on the variance and Chebyshev's inequality it follows that

$$\mathbb{P}_{B_n,\lambda}[|\mathbf{X}| \in (\mathbb{E}_{B_n,\lambda}|\mathbf{X}| - n^{4/5}, \mathbb{E}_{B_n,\lambda}|\mathbf{X}| + n^{4/5})] \geqslant 1 - \frac{1}{n^{1/10}}.$$

Since there are at most $\lfloor 2n^{4/5} \rfloor$ integers in the interval $(\mathbb{E}_{B_n,\lambda}|\mathbf{X}| - n^{4/5}, \mathbb{E}_{B_n,\lambda}|\mathbf{X}| + n^{4/5})$ we may pick some k in this interval so that

$$\mathbb{P}_{B_n,\lambda}[|\mathbf{X}| = k] = \frac{\lambda^k \hat{Z}_{B_n}(k)}{Z_{B_n}(\lambda)} \geqslant \frac{1 - n^{-1/10}}{\lfloor 2n^{4/5} \rfloor} \geqslant \frac{1}{n}.$$

It follows that

$$\hat{Z}_{B_n}(k) \geqslant \frac{1}{n} \frac{1}{\lambda^k} Z_{B_n}(\lambda) \geqslant \frac{1}{n} \frac{1}{\lambda^k}, \tag{15}$$

where we used the trivial bound $Z_{B_n}(\lambda) \geqslant 1$. Note that by our choice of λ we have

$$\mathbb{E}_{B_n,\lambda}|\mathbf{X}| \geqslant (1 + o_d(1)) \frac{\log(2/\sqrt{3}) \cdot d}{2^d} \cdot n$$

by Theorem 2. Letting $\alpha = k/n$, it follows that by our choice of k we have $\alpha \geqslant (1 + o_{n,d}(1))((\log(2/\sqrt{3}) \cdot d)/2^d)$. It then follows from (15) that

$$\frac{1}{\alpha n} \log \frac{\hat{Z}_{B_n}(k)}{n^k/k!} \geqslant \log \alpha - \log \lambda - 1 + o_n(1)$$

$$\geqslant -(1 + o_{n,d}(1)) \log(2/\sqrt{3}) \cdot d.$$

Taking $n \to \infty$ and recalling Lemma 11 proves the theorem. □

4.1. Comparison of Theorem 5 to the cell model lower bound.

Given a lattice packing of B_n with $k = c_1 d \cdot 2^{-d}(1 - \varepsilon)^d n$ spheres of radius $r_d/(1 - \varepsilon)$ (and thus density $\Theta(d \cdot 2^{-d})$), construct the Voronoi diagram around the centers of the packing. Around each center, place a copy of its Voronoi cell scaled down by a factor ε. If the centers are allowed to move arbitrarily within their respective shrunken cells, they still form a packing of spheres of radius r_d. The density of such a packing is $c_1(1 - \varepsilon)^d d 2^{-d}$, and so if we take $\varepsilon = c_2/d$, then the resulting packing still has density $\sim c_1 e^{-c_2} d \cdot 2^{-d}$. The probability that a random set of k points in B_n is such a configuration is the probability that each of the k shrunken cells contain exactly one of k uniformly random points, that is:

$$\frac{k!}{n^k} \varepsilon^{dk} (n/k)^k$$

since the volume of each shrunken Voronoi cell is $n/k \cdot \varepsilon^d$. This gives

$$\hat{Z}_{B_n}(k) \geqslant \varepsilon^{dk} (n/k)^k,$$

and so with $\alpha = k/n \sim c_1 e^{-c_2} d \cdot 2^{-d}$,

$$\frac{1}{\alpha n} \log \frac{\hat{Z}_{B_n}(k)}{n^k/k!} \geqslant \frac{1}{\alpha n} \log \frac{\varepsilon^{dk}}{e^k} = -(1 + o_d(1))d \log d,$$

which is considerably smaller (of a different asymptotic order) than the bound in Theorem 5.

Acknowledgments

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