

Estimates of the optimal density of sphere packings in high dimensions

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The problem of finding the asymptotic behavior of the maximal density ϕ_{\max} of sphere packings in high Euclidean dimensions is one of the most fascinating and challenging problems in discrete geometry. One century ago, Minkowski obtained a rigorous lower bound on ϕ_{\max} that is controlled asymptotically by $1/2^d$, where d is the Euclidean space dimension. An indication of the difficulty of the problem can be garnered from the fact that exponential improvement of Minkowski's bound has proved to be elusive, even though existing upper bounds suggest that such improvement should be possible. Using a statistical-mechanical procedure to optimize the density associated with a "test" pair correlation function and a conjecture concerning the existence of disordered sphere packings [S. Torquato and F. H. Stillinger, *Exp. Math.* **15**, 307 (2006)], the putative exponential improvement on ϕ_{\max} was found with an asymptotic behavior controlled by $1/2^{(0.77865\cdots)d}$. Using the same methods, we investigate whether this exponential improvement can be further improved by exploring other test pair correlation functions corresponding to disordered packings. We demonstrate that there are simpler test functions that lead to the same asymptotic result. More importantly, we show that there is a wide class of test functions that lead to precisely the same putative exponential improvement and therefore the asymptotic form $1/2^{(0.77865\cdots)d}$ is much more general than previously surmised. This class of test functions leads to an optimized average kissing number that is controlled by the same asymptotic behavior as the one found in the aforementioned paper. © 2008 American Institute of Physics.
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I. INTRODUCTION

A collection of congruent spheres in d -dimensional Euclidean space \mathbb{R}^d is called a *sphere packing* if no two spheres overlap. Although the practical relevance of sphere packings in high Euclidean dimensions was appreciated by Shannon in 1948,¹ there has been a resurgence of interest in such problems in both the physical and mathematical sciences.^{2–11} Shannon showed that the optimal way of sending digital signals over noisy channels corresponds to the densest sphere

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packing in a high dimensional space.¹ These “error-correcting” codes underlie a variety of systems in digital communications and storage.¹² Physicists have investigated sphere packings in high dimensions to gain insight into classical ground and glassy states of matter as well as phase behavior in lower dimensions.^{8,9,13–15} Understanding the symmetries and other mathematical properties of the densest packings in arbitrary dimension is a problem of long-standing interest in discrete geometry and number theory.^{4,5,12,16,17}

The *packing density* or simply density ϕ of a sphere packing is the fraction of space \mathbb{R}^d covered by the spheres. We will call

$$\phi_{\max} = \sup_{P \subset \mathbb{R}^d} \phi(P) \quad (1)$$

the *maximal density*, where the supremum is taken over all packings that exist in \mathbb{R}^d .¹⁸ The set of (Bravais) lattice packings is a subset of the set of sphere packings in \mathbb{R}^d .¹⁹ In such a packing, space can be partitioned into identical regions called *fundamental cells*, each of which contains just one sphere center. Nonlattice packings include periodic packings (more than one sphere per fundamental cell) as well as disordered packings.²⁰

The sphere packing problem seeks to answer the following question: Among all packings of congruent spheres, what is the maximal packing density ϕ_{\max} , i.e., largest fraction of \mathbb{R}^d covered by the spheres, and what are the corresponding arrangements of the spheres?^{12,17} For arbitrary d , the sphere packing problem is notoriously difficult to solve. Exact solutions are only known for the first three space dimensions.⁵ For $4 \leq d \leq 9$, the densest known packings of congruent spheres are lattice packings. For example, the “checkerboard” lattice D_d , which is the d -dimensional generalization of the fcc lattice (densest packing in \mathbb{R}^3), is believed to be optimal in \mathbb{R}^4 and \mathbb{R}^5 . The remarkably symmetric E_8 and Leech lattices in \mathbb{R}^8 and \mathbb{R}^{24} , respectively, are most likely the densest packings in these dimensions.¹¹ However, for sufficiently large d , lattice packings are most likely not the densest, but it becomes increasingly difficult to find dense packing constructions as d increases.²¹ For large d , the best that one can do theoretically is to devise the upper and lower bounds on ϕ_{\max} .

The upper and lower bounds on the maximal density ϕ_{\max} exist in all dimensions.¹² Minkowski²² proved that the maximal density ϕ_{\max}^L among all Bravais lattice packings for $d \geq 2$ satisfies the lower bound

$$\phi_{\max}^L \geq \frac{\zeta(d)}{2^{d-1}}, \quad (2)$$

where $\zeta(d) = \sum_{k=1}^{\infty} k^{-d}$ is the Riemann zeta function. The large- d asymptotic behavior of the *non-constructive* Minkowski lower bound is controlled by 2^{-d} . Since 1905, many extensions and generalizations of (2) have been derived,¹² but none of them has improved upon the dominant exponential term 2^{-d} . The best currently known rigorous lower bound on ϕ_{\max}^L ,

$$\phi_{\max}^L \geq \frac{2(d-1)\zeta(d)}{2^d} \quad (3)$$

was obtained by Ball.²³ Interestingly, the density of a *saturated* packing of congruent spheres in \mathbb{R}^d for all d satisfies the lower bound²⁴

$$\phi \geq \frac{1}{2^d}, \quad (4)$$

and thus has the same dominant exponential term Minkowski’s bound (2). A *saturated packing* of congruent spheres of unit diameter and density ϕ in \mathbb{R}^d has the property that each point in space lies within a unit distance from the center of some sphere. The lower bound (4) is not stringent for a saturated packing and hence is improvable, as we will see.

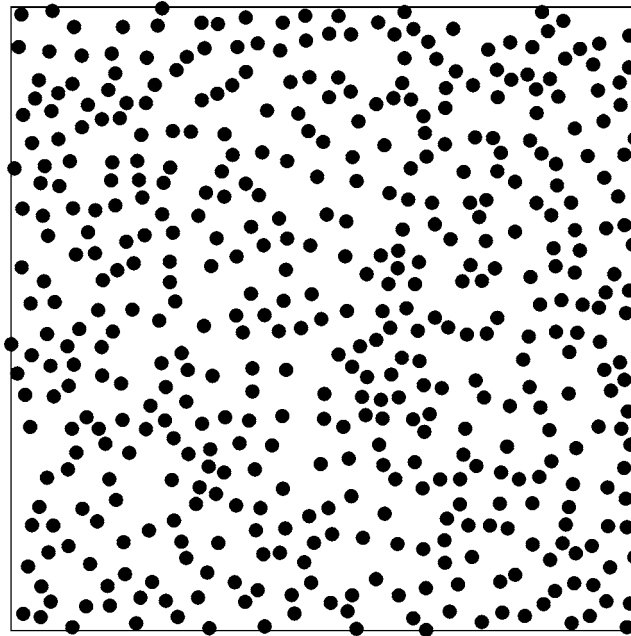


FIG. 1. A configuration of 468 particles of a ghost RSA packing in \mathbb{R}^2 at a density very near its maximal density of 0.25. This was generated using a Monte Carlo procedure within a square fundamental cell under periodic boundary conditions. Note that the packing is clearly unsaturated and there are no contacting particles.

Rogers^{16,17} found upper bounds on the maximal density ϕ_{\max} that asymptotically becomes $d/(2^{d/2}e)$. Kabatiansky and Levenshtein²⁵ found an even stronger bound, which in the limit $d \rightarrow \infty$ yields $\phi_{\max} \leq 2^{-0.5990d(1+o(1))}$. Cohn and Elkies⁴ obtained and computed linear programming upper bounds that improve Rogers' upper bound for dimensions 4–36. Cohn and Kumar¹¹ used these techniques to prove that the E_8 and Leech lattices are the unique densest lattices in \mathbb{R}^8 and \mathbb{R}^{24} , respectively. They also proved that no sphere packing in \mathbb{R}^{24} can exceed the density of the Leech lattice by a factor of more than $1 + 1.65 \times 10^{-30}$.

A recent study⁶ proved that there exists a disordered packing construction in \mathbb{R}^d , called the “ghost” random sequential addition (RSA) packing,²⁶ with a maximal density that achieves the saturation lower bound (4) for any d . The n -particle correlation function g_n (defined below) for this packing for any $n \geq 1$ was obtained analytically for all allowable densities and d . Interestingly, this packing is *unsaturated* (see Fig. 1) and yet has a maximal density 2^{-d} , suggesting that there exist disordered saturated packings with densities that exceed the saturation lower bound (4) or bound (2). Indeed, the maximal saturation density of the standard disordered RSA packing²⁷ apparently scales as $d/2^d$ for large d ,¹⁰ which has the same asymptotic behavior as Ball's lower bound (3). Spheres in both the ghost and standard RSA packings cannot form interparticle contacts, which appears to be a crucial attribute to obtain exponential improvement on Minkowski's bound,⁷ as we discuss below.

Torquato and Stillinger⁷ used a conjecture concerning the existence of disordered sphere packings and an optimization procedure that maximizes the density associated with a “test” pair correlation function $g_2(\mathbf{r})$ to provide the putative exponential improvement on Minkowski's 100-year-old bound on ϕ_{\max} (see Sec. II for details). The asymptotic behavior of the conjectural lower bound is controlled by $2^{-(0.77865 \dots)d}$. Moreover, this lower bound always lies below the density of the densest known packings for $3 \leq d \leq 56$, but, for $d > 56$, it can be larger than the densities of the densest known arrangements, all of which are ordered. These results counterintuitively suggest that the densest packings in sufficiently high dimensions may be disordered rather than periodic, implying the existence of disordered classical ground states for some continuous potentials. In addition, a *decorrelation* principle for disordered packings was identified in Ref. 7,

which states that *unconstrained* correlations in disordered sphere packings vanish asymptotically in high dimensions and that the n -particle correlation function g_n for any $n \geq 3$ can be inferred entirely (up to some small error) from a knowledge of the number density ρ and pair correlation function $g_2(\mathbf{r})$. This decorrelation principle,²⁸ among other things, provides justification for the conjecture used in Ref. 7, and is vividly exhibited by the exactly solvable ghost RSA packing process⁶ as well as by computer simulations in high dimensions of the maximally random jammed state⁹ and the standard RSA packing process.¹⁰

In this paper, we investigate whether the putative exponential improvement of Minkowski's lower bound found in Ref. 7 can be further improved by exploring other test pair correlation functions. We will show that there are simpler test functions that lead to the same asymptotic result. More importantly, we will demonstrate that there is a wide class of test functions that lead to the same exponential improvement as in Ref. 7.

II. PRELIMINARIES AND OPTIMIZATION PROCEDURE

A packing of congruent spheres of unit diameter is simply a point process in which any pair of points cannot be closer than a unit distance from one another.⁷ A particular configuration of a point process in \mathbb{R}^d is described by the "microscopic" density,

$$n(\mathbf{r}) = \sum_{i=1}^{\infty} \delta(\mathbf{r} - \mathbf{x}_i). \quad (5)$$

This distribution can be interpreted in a probabilistic sense,⁷ which is particularly useful for the arguments we will present, even in the limit in which no explicit randomness is present, as in the case in which the spheres are arranged on the sites of a (Bravais) lattice. We define the n -particle density as the ensemble average

$$\rho_n(\mathbf{r}_1, \dots, \mathbf{r}_n) = \left\langle \sum_{i_1 \neq i_2 \neq \dots \neq i_n} \delta(\mathbf{r}_1 - \mathbf{x}_{i_1}) \dots \delta(\mathbf{r}_n - \mathbf{x}_{i_n}) \right\rangle, \quad (6)$$

which is a non-negative quantity. Henceforth, we will assume that the random process is translationally invariant, i.e., statistically homogeneous. It follows that there is no preferred origin in the packing and thus the n -particle densities $\rho_n(\mathbf{r}_{12}, \mathbf{r}_{13}, \dots, \mathbf{r}_{1n})$ only depend on relative displacements, where $\mathbf{r}_{1j} \equiv \mathbf{r}_j - \mathbf{r}_1$. In particular, the one-particle density $\rho_1(\mathbf{r}) = \langle \delta(\mathbf{r} - \mathbf{x}_1) \rangle = \rho$ is a constant called the *number (center) density*. The packing density ϕ defined earlier is related to the number density ρ for spheres of unit diameter via the relation

$$\phi = \rho v_1(1/2), \quad (7)$$

where $v_1(r) = \pi^{d/2} r^d / \Gamma(d/2 + 1)$ is the volume of a sphere of radius r . The surface area of such a sphere is $s_1(r) = 2\pi^{d/2} r^{d-1} / \Gamma(d/2)$. If we divide ρ_n by ρ^n , we get the n -particle correlation function $g_n(\mathbf{r}_{12}, \mathbf{r}_{13}, \dots, \mathbf{r}_{1n})$, which clearly is also a non-negative function. As will become clear shortly, the *pair correlation* function $g_2(\mathbf{r}_{12})$ has particular importance to us. If the point process is additionally rotationally invariant (i.e., the packing is statistically homogeneous and isotropic), the pair correlation function $g_2(r)$ depends only on the distance $r \equiv |\mathbf{r}|$.

In Ref. 2, g_2 -invariant processes were examined in order to gain insights about the nature of disordered sphere packings. A g_2 -invariant process is one in which a given non-negative pair correlation $g_2(\mathbf{r})$ function has a fixed functional form for all \mathbf{r} over the range of densities $0 \leq \phi \leq \phi_*$. The terminal density ϕ_* is the maximum achievable density for the g_2 -invariant process subject to satisfaction of certain necessary conditions on the pair correlation. In particular, they considered those test $g_2(r)$'s that are distributions on \mathbb{R}^d depending only on the radial distance r . For any test $g_2(r)$ associated with a packing, i.e., $g_2(r) = 0$ for $r < 1$, they maximized the corresponding density ϕ , i.e.,

$$\max \phi \quad (8)$$

subject to the following two conditions:

$$g_2(r) \geq 0 \quad \text{for all } r, \quad (9)$$

$$S(k) = 1 + \rho(2\pi)^{d/2} \int_0^\infty dr r^{d-1} \frac{J_{d/2-1}(kr)}{(kr)^{d/2-1}} [g_2(r) - 1] \geq 0 \quad \text{for all } k. \quad (10)$$

Condition (10) states that the structure factor $S(k)$ [trivially related to the Fourier transform of $g_2(r) - 1$]²⁹ must also be non-negative for all wavenumbers. It is a known necessary condition on the existence of a point process,^{2,30} but it is generally not sufficient.³¹

Recently, Torquato and Stillinger⁷ conjectured that a disordered sphere packing in \mathbb{R}^d at number density ρ exists for sufficiently large d if and only if the conditions (9) and (10) are satisfied. The maximum achievable density is the terminal density ϕ_* , which then implies the lower bound

$$\phi_{\max} \geq \phi_*. \quad (11)$$

There is mounting evidence to support this conjecture. First, the aforementioned decorrelation principle states that unconstrained correlations in disordered sphere packings vanish asymptotically in high dimensions and that the g_n for any $n \geq 3$ can be inferred entirely from a knowledge of ρ and g_2 . Second, other necessary conditions on g_2 , such as the Yamada condition³² as well as others,⁷ appear to only have relevance in very low dimensions. Third, one can recover the form of known rigorous bounds [see (2) and (3)] for specific test g_2 's when the conjecture is invoked. Finally, in these two instances, configurations of disordered sphere packings on the torus have been numerically constructed with such g_2 in low dimensions for densities up to the terminal density.^{33,34}

Interestingly, the optimization problem defined above is the *dual* of the infinite-dimensional linear program (LP) devised by Cohn and Elkies^{3,4} to obtain upper bounds on the maximal packing density. In particular, let $f(r)$ be a radial function in \mathbb{R}^d such that

$$\begin{aligned} f(r) &\leq 0 \quad \text{for } r \geq 1, \\ \tilde{f}(k) &\geq 0 \quad \text{for all } k. \end{aligned} \quad (12)$$

Then the number density ρ is bounded from above by

$$\min \frac{f(0)}{2^d \tilde{f}(0)}. \quad (13)$$

The radial function $f(r)$ can be physically interpreted to be a *pair potential*. The fact that its Fourier transform must be non-negative for all k is a well-known stability condition for many-particle systems with pairwise interactions.³⁵ We see that whereas the LP problem specified by (8)–(10) utilizes information about pair correlations, its dual program (12) and (13) uses information about pair interactions. As noted in Ref. 7, even if there does not exist a sphere packing with g_2 satisfying conditions (9) and (10), the terminal density ϕ_* can never exceed the Cohn–Elkies upper bound. Every LP has a dual program³⁶ and when an optimal solution exists, there is no *duality gap* between the upper-bound and lower-bound formulations. Recently, Cohn and Kumar³⁷ proved that there is no duality gap.

By means of the aforementioned LP problem and conjecture concerning the existence for a certain test function g_2 , it was found in Ref. 7 that in the limit $d \rightarrow \infty$,

$$\phi_{\max} \geq \phi_* \sim 2^{-(3/2)d + (1/\ln 2)(d/2) + 2.12497 \cdots d^{1/3} + (1/6)\log_2 d + \log_2(3.2761 \cdots)}, \quad (14)$$

where the terms neglected are monotonically decreasing with d . The first term in the series provides the putative exponential improvement of Minkowski's lower bound (2). In the following, we will be interested mainly in the exponential improvement of Minkowski's lower bound, and so we simplify the right-hand side of (14) by writing it as

$$\phi_* \sim 2^{-((3/2) - (1/2 \ln 2))d} = 2^{-0.77865 \cdots d}. \quad (15)$$

This is not to be intended as an asymptotic expansion of ϕ_* in the sense of Poincaré (the ratio of the right-hand side to the left-hand side does not go to unity when $d \rightarrow \infty$); however, it is an asymptotic expansion in such sense for $\log_2 \phi_*$.

In what follows, we will show that we can obtain a conjectural lower bound asymptotically equal to (14) with a simpler test function. Then we will demonstrate that the requirement of hyperuniformity³⁰ in Ref. 7 is actually a necessary condition that arises only from the optimization procedure. A point process is called *hyperuniform* if the structure factor²⁹ vanishes in the limit $\mathbf{k} \rightarrow \mathbf{0}$, i.e., infinite wavelength density fluctuations vanish; see Ref. 30. Finally, we will show some examples of how enlarging the space of test functions where the optimization is performed does not change the asymptotic *exponential* behavior, although nonexponential improvement is found. Although these results do not constitute a proof of lower bounds, they strongly suggest that an estimate of the asymptotic behavior of the solutions to the LP lower-bound problem can be achieved and that physical intuition is gained about the spatial structures they describe.

III. STEP PLUS DELTA FUNCTION REVISITED

Following Torquato and Stillinger,⁷ we choose the following test $g_2(r)$:

$$g_2(r) = \Theta(r-1) + \frac{Z}{s_1(1)\rho} \delta(r-1). \quad (16)$$

Here, the parameter Z has the interpretation of the average kissing number. The structure factor becomes

$$S(k) = 1 - 2^{d/2} \Gamma\left(1 + \frac{d}{2}\right) \frac{J_{d/2}(k)}{k^{d/2}} 2^d \phi + 2^{d/2-1} \Gamma\left(\frac{d}{2}\right) \frac{J_{d/2-1}(k)}{k^{d/2-1}} Z \equiv 1 - a(k)2^d \phi + b(k)Z, \quad (17)$$

which defines the functions a, b . The terminal density is defined by the linear program (8)–(10). Z is then a free parameter to be optimized appropriately. A positive value of Z requires contacting spheres, which is to be contrasted with the ghost RSA process, depicted in Fig. 1, in which spheres can never touch and whose density cannot exceed $1/2^d$. It was shown⁷ that optimizing Z leads to a density that surpasses $1/2^d$.

Unlike Torquato and Stillinger,⁷ here we do not impose hyperuniformity^{29,30} (requiring the structure factor to vanish at $k=0$) to simplify the optimization. Moreover, we are also interested in finding the largest average kissing number Z that (for a given d) satisfies the constraints. In this latter case, it is ϕ that must be chosen appropriately. These are two infinite-dimensional LP problems.

There is a graphical construction that will help us look for such points and that will be helpful also in cases where more parameters are to be varied. For any given k , the set of allowed points in the (ϕ, Z) plane [i.e., those for which $S(k) \geq 0$] is the half plane above (below) the line $1 - a(k)2^d \phi + b(k)Z = 0$ for positive (negative) a . Upon changing k by a small step to $k + \Delta$, we repeat the construction and find the intersection of the two half-planes. By letting k vary over the positive reals and letting $\Delta \rightarrow 0$, we find a limiting finite, convex region \mathcal{B} which gives the allowed values of ϕ, Z . This region is the set internal to the curve obtained by solving the equations

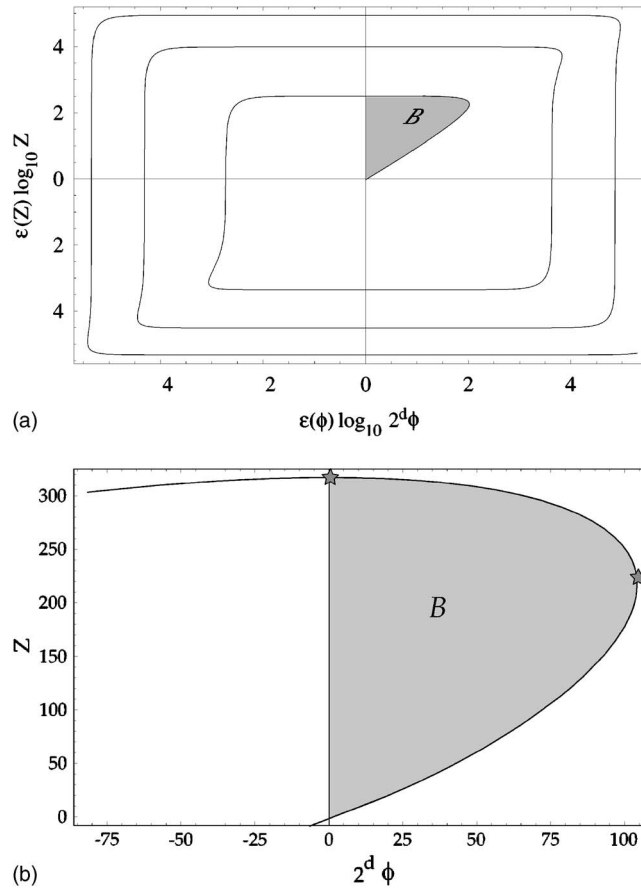


FIG. 2. (Top panel) For $d=16$, the set B of allowed packing densities and kissing numbers. The rightmost point is the maximal packing density ϕ_* and its corresponding kissing number Z_* . The topmost point is the maximal kissing number Z_{**} which corresponds to packing density $\phi_{**}=0$. (Bottom panel) As in the top panel, the region B of allowed packing densities and kissing numbers for $d=16$. For convenience in plotting, the horizontal and vertical axes represent the functions $\epsilon(\phi) \log_{10}(2^d \phi)$, and $\epsilon(Z) \log_{10}(Z)$, where $\epsilon(x) = \text{sign } x$, respectively (although in this way the small region $|2^d \phi| < 1, |Z| < 1$ had to be left out of the graph). This figure shows how the solution of the equations $S(k, \phi, Z) = 0, \partial S(k, \phi, Z) / \partial k = 0$ for varying k form an ever-growing spiral in which the allowed region B is completely contained. So this geometrical construction proves that every point in B are solutions to the LP problem $S(k, \phi, Z) \geq 0, \phi \geq 0, Z \geq 0$ for every $k \geq 0$.

$$S(k, \phi, Z) = 0, \quad \frac{\partial}{\partial k} S(k, \phi, Z) = 0, \tag{18}$$

with respect to ϕ, Z . This is depicted in Fig. 2. It is not difficult to prove that the region B is indeed internal to the entire spiral. It will suffice to observe that the distance of a point on the spiral from the origin is a monotonically increasing function (for sufficiently large k).

Now the terminal density ϕ_* is the x -component of the rightmost point in B . Analogously the y -component of the topmost point in B gives the predicted terminal kissing number Z_{**} .

The terminal density is found at the first zero of $b(k)$, which is located at the first zero of the Bessel function of order $d/2 - 1$. As customary, we call this number $j_{d/2-1,1}$. The value of (ϕ_*, Z_*) is then found by finding the point on the spiral corresponding to $k = j_{d/2,1}$:

$$\phi_* = \frac{2^{-d}}{a(j_{d/2-1,1})} = 2^{-3d/2} \frac{(j_{d/2-1,1})^{d/2}}{\Gamma(1 + d/2) J_{d/2}(j_{d/2-1,1})}, \tag{19}$$

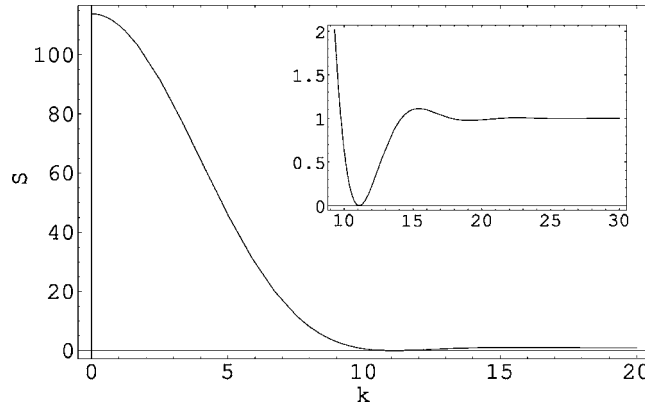


FIG. 3. The structure factor for the terminal density $\phi_* = 0.0046692$, $Z_* = 217.121$ in $d = 16$. Notice the zero at $k^* = j_{7,1} = 11.086 \dots$ and the rapid asymptoting to the value $S(\infty) = 1$.

$$Z_* = \frac{a'(j_{d/2-1,1})}{b'(j_{d/2-1,1})a(j_{d/2-1,1})} = \frac{a'(j_{d/2-1,1})}{b'(j_{d/2-1,1})} 2^d \phi_* \quad (20)$$

By using the asymptotic formulas, valid for large ν ,

$$j_{\nu,1} = \nu + 1.85576 \dots \nu^{1/3} + \mathcal{O}(\nu^{-1/3}), \quad (21)$$

$$J_\nu(j_{\nu-1,1}) = -J'_{\nu-1}(j_{\nu-1,1}) = 1.11310 \dots \nu^{-2/3} + \mathcal{O}(\nu^{-4/3}), \quad (22)$$

we find

$$\phi_* \approx 2^{-(3/2)d + (1/\ln 2)(d/2) + 2.12497 \dots d^{1/3}} \sim 2^{-(0.77865 \dots)d}. \quad (23)$$

Notice that this is the same case that was treated in Ref. 7 but there hyperuniformity was imposed and the Minkowski bound was recovered. Here, we are *not imposing* hyperuniformity and the resulting terminal structure factor is not hyperuniform. The form of $S(k)$ at the terminal point ϕ_*, Z_* is given in Fig. 3. Notice that the first zero is at $k = j_{d/2-1,1} \approx d/2$. This can be interpreted as the appearance of a structure with length scale $\ell \sim 1/d$ in the system at large d . However, since a sphere packing corresponding to such a $S(k)$ could not be hyperuniform, it cannot be a Bravais lattice.

Following Ref. 7, we checked whether the Yamada condition³² on the number variance is satisfied by the pair correlation (16). As in Ref. 7, we found a violation only for $d = 1$.

The terminal kissing number is given by the topmost point in \mathcal{B} which is point k^{**} , where $a(k^{**}) = 0$. It can be easily proved that $b'(k^{**}) = 0$ as well so that

$$Z_{**} = -\frac{1}{b(j_{d/2,1})} \sim 2^{((1/\ln 2) - 1)d/2}, \quad (24)$$

with an associated density $\phi_{**} = 0$, which is a singular point. The equality is valid in any dimension and the asymptotic result applies for large d . One must regard the singular zero-density limit point on the top boundary of \mathcal{B} (and perhaps a positive small interval in its vicinity) with caution because such a zero-density state may not be realizable by a packing. However, we should note that the optimal kissing number Z_{**} has the same asymptotic form as the kissing number associated with the maximal density ϕ_* ,⁷ which to our knowledge has no obvious realizability problems. This means that, except for a small positive density interval around zero, most of the upper boundary of \mathcal{B} for positive densities is apparently realizable.

IV. STEP PLUS DELTA FUNCTION WITH A GAP

This case was analyzed in Ref. 7 before by imposing hyperuniformity. Here we show that in order to find the terminal density, one does not need to impose hyperuniformity²⁹ from the beginning but rather that it arises as a necessary condition from the optimization procedure. We will show that the same asymptotic behavior of the terminal density found in the previous example is obtained (modulo nonexponential prefactors).

We choose the test function

$$g_2(r) = \Theta(r - (1 + \sigma)) + \frac{Z}{s_1(1)\rho} \delta(r - 1), \quad (25)$$

depending on two parameters Z, σ and the density of centers ρ . Performing the integrals gives the corresponding structure factor

$$S(k) = 1 - a((1 + \sigma)k)2^d(1 + \sigma)^d \phi + b(k)Z, \quad (26)$$

where the functions a, b were defined in the previous section. Again we look for the rightmost point in the set, which is now given by

$$\phi_* = \frac{2^{-d}}{(1 + \sigma)^d a((1 + \sigma)j_{d/2-1,1})} \quad (27)$$

$$Z_* = \frac{(1 + \sigma)a'((1 + \sigma)k)}{b'(j_{d/2-1,1})a((1 + \sigma)j_{d/2-1,1})}. \quad (28)$$

We now need to maximize the value of ϕ_* over σ . Clearly, we can increase σ to increase ϕ_* indefinitely until $a((1 + \sigma)j_{d/2-1,1})$ becomes zero, namely, when $(1 + \sigma)j_{d/2-1,1} = j_{d/2,1}$, which gives $\sigma \sim 2/d$. The prefactor goes to a constant: $(1 + \sigma)^d \sim (1 + 2/d)^d \sim e^2$ and does not change the asymptotic dependence on d . This would suggest that the density can be increased without bound by adjusting the other parameters. This is not the case, however, since when we increase σ we encounter the first “global” obstacle [by which we mean at wavenumbers k far from the first zero of $b(k)$, which was setting the relevant k scales up to now] at the value of σ when $(1 + \sigma)^d 2^d \phi_* = Z_* - 1$. Notice that $a(0) = b(0) = 1$ and both functions decrease monotonically until their first zeros; here we have $S(0) = 1 - (1 + \sigma)^d 2^d \phi_* + Z_* = 0$ and any further increase of σ would make $S(0) < 0$. Thus, hyperuniformity has arisen as an optimality condition. Of course one should make sure that there is not a disconnected region in the parameter space (σ, ϕ, Z) with better terminal density ϕ_* but where hyperuniformity does not hold. We have searched the parameter space by discretizing the relevant range of k and solving, using MATHEMATICA, the LP problem (8)–(10). We have not been able to find another allowed region of the parameters disconnected from the previous one.

Henceforth, we assume that the global terminal value ϕ_* is indeed obtained by imposing hyperuniformity²⁹ and maximizing with respect to the remaining parameters (the two operations can be performed in any order). We notice that now we have reduced the problem to the case that has been analyzed in Ref. 7. We will not repeat that analysis here but refer the reader to that paper. It is important to observe that in Ref. 7, the resultant asymptotic scaling laws for the terminal density ϕ_* and the kissing number Z_* coincide with the ones presented in the previous section, where we found $\phi_* \sim 2^{-(0.77865 \dots)d}$ and $Z_* \sim 2^{0.22134 \dots d}$. Although the nonexponential terms are different from those in the previous section, it is remarkable that the same exponential scaling laws arise for two different cases. This strongly suggests that a large class of test functions can possess this asymptotic behavior. With this in mind, we go on to analyze the next case in which the test pair-correlation function consists of a hard core with two delta functions and a gap.

V. STEP PLUS TWO DELTA FUNCTIONS WITH A GAP

In this section, we find the solution of the optimization problem (8)–(10) for the family of pair-correlation functions $g_2(r)$ composed of unit step function plus a gap and two delta functions, one at contact and the other at the end of the gap:

$$g_2(r) = \Theta(r - (1 + \sigma)) + \frac{Z_2}{s(1)\rho} \delta(r - 1) + \frac{Z_1}{s(1 + \sigma)\rho} \delta(r - (1 + \sigma)). \quad (29)$$

This family depends on three parameters σ, Z_1, Z_2 and we need to optimize them in order to find the optimal terminal density ϕ_* . The structure factor is

$$S(k) = 1 + Z_2 2^{d/2-1} \Gamma(d/2) \frac{J_{d/2-1}(k)}{k^{d/2-1}} + Z_1 2^{d/2-1} \Gamma(d/2) \frac{J_{d/2-1}(k(1 + \sigma))}{(k(1 + \sigma))^{d/2-1}} - \phi \Gamma(d/2 + 1) (1 + \sigma)^{d/2} \frac{J_{d/2}((1 + \sigma)k)}{(k(1 + \sigma))^{d/2}} \quad (30)$$

$$\equiv 1 + Z_2 c(k) + Z_1 b(k) - (1 + \sigma)^{d/2} \phi a(k), \quad (31)$$

where the last line defines the functions a, b, c . Notice that $a(0) = b(0) = c(0) = 1$ and $|a(k)|, |b(k)|, |c(k)| \leq 1$ follow from the properties of the Bessel functions. It is also convenient to reabsorb the factor $(1 + \sigma)^{d/2}$ in the definition of ϕ , i.e., $(1 + \sigma)^{d/2} \phi \rightarrow \phi$. We will restore the proper units at the end of the calculation. The solution of this optimization problem for arbitrary d is a formidable task. However, guided by the results of the previous section, we assume we can find an improvement on the previous bound even after imposing hyperuniformity.

Therefore, we fix the value of $Z_2 = \phi - Z_1 - 1$ and are left with the other two parameters to optimize. Inserting this value of Z_2 in (31), we find the reduced optimization problem

$$S(k) = (1 - c(k)) - (a(k) - c(k))\phi + (b(k) - c(k))Z_1 \geq 0. \quad (32)$$

By using the fact that $c(k) \leq 1$, we might as well study the optimization problem

$$S^{(1)}(k, \sigma, \phi, Z_1) \equiv \frac{S(k)}{1 - c(k)} \equiv 1 - \alpha(k)\phi + \beta(k)Z_1 \geq 0, \quad (33)$$

$$\alpha(k) = \frac{a(k) - c(k)}{1 - c(k)}, \quad (34)$$

$$\beta(k) = \frac{b(k) - c(k)}{1 - c(k)}. \quad (35)$$

Formally, this problem is analogous to the previous case with one delta function with gap and can be studied in the very same fashion. The process of having solved for Z_2 and changed the functions a, b to α, β can be thought of as a *renormalization* process that allows to *integrate out* one delta function to reduce the problem to a simpler one.

The mathematical problem of finding the terminal fraction is formally identical to that of the previous section, although the constitutive functions α, β are more complicated. However, as long as a numerical analysis is concerned this does not present further difficulties.

We proceed in the following way: for a fixed σ we find the rightmost point of allowed region, $\phi_*(\sigma), Z_{1,*}(\sigma)$, by finding the first zero of $\beta(k)$, call it k^* ,

$$\phi_*(\sigma) = \frac{1}{\alpha(k^*)}, \quad (36)$$

TABLE I. Estimates of the maximal densities for selected dimensions up to $d=150$. ϕ_{bk} is the densest known packing, ϕ_{CE} is the upper bound of Cohn and Elkies, $\phi_{1,*}$ is the terminal density for a single delta function, and $\phi_{2,*}$ for two delta functions.

d	ϕ_{bk}	ϕ_{CE}	$\phi_{*,1}$	$\phi_{*,2}$
3	0.740 49	0.779 82	0.576 65	0.633 06
4	0.616 85	0.647 74	0.425 26	0.478 85
5	0.465 27	0.525 06	0.305 91	0.354 37
6	0.372 95	0.417 76	0.213 60	0.249 66
7	0.295 30	0.327 57	0.147 13	0.179 91
8	0.253 67	0.253 67	0.099 85	0.124 67
12	0.049 45	0.083 84	0.019 15	0.0257 21
15	0.016 85	0.034 33	0.005 16	0.007 22
19	0.0041 21	0.0098 85	0.0008 45	0.0012 33
24	0.001 93	0.001 93	8.24×10^{-5}	0.0001 25
31	1.18×10^{-5}	1.93×10^{-4}	2.91×10^{-6}	4.57×10^{-6}
36	6.14×10^{-7}	3.59×10^{-5}	2.57×10^{-7}	4.13×10^{-7}
56	2.33×10^{-11}	...	1.25×10^{-11}	2.13×10^{-11}
60	2.97×10^{-13}	...	1.67×10^{-12}	2.87×10^{-12}
64	1.33×10^{-13}	...	2.22×10^{-13}	3.83×10^{-13}
80	1.12×10^{-16}	...	6.52×10^{-17}	1.15×10^{-16}
100	2.28×10^{-21}	4.11×10^{-21}
150	8.44×10^{-39}	...	1.27×10^{-32}	2.30×10^{-32}

$$Z_{1,*}(\sigma) = \frac{\alpha'(k^*)}{\beta'(k^*)\alpha(k^*)}. \quad (37)$$

We then maximize the value of $\phi_*(\sigma)$ with respect to variations of σ . Generically, increasing σ increases the value of ϕ_* until a positivity condition is violated (for small k). It turns out that the first condition to be violated is $S^{(1)}(0) \geq 0$. So in practice we find the terminal value of σ by solving the equation

$$S^{(1)}(0, \sigma, \phi_*(\sigma), Z_{1,*}(\sigma)) = 0, \quad (38)$$

with respect to σ . Notice that this is now a “strong” hyperuniformity requirement, since $S^{(1)}(k) \sim k^2$ near the origin implies $S(k) \sim k^4$ near the origin, since $1 - c(k) \sim k^2$. We are tempted to conjecture that this is a universal feature: adding more delta functions to g_2 and solving the LP problem, we obtain structure factors $S(k)$ that become increasingly flatter at the origin. Hence, at least in this respect, the structure factor looks increasingly similar to that of a lattice.

As can be seen from Table I and Fig. 4 (here the proper normalization for ϕ has been restored), the improvement on the previous bound is relevant but the asymptotic exponent is the same. Analytically, it is not difficult to obtain the rate of exponential decay (dictated mainly by the Stirling expansion of the gamma functions and the scaling of the first zero of β with d for large d), which turns out to be the *same* as the previous cases, namely,

$$\phi_* \sim 2^{-(3/2 - 1/2 \ln 2)d}. \quad (39)$$

It is plausible, therefore, that the incorporation of any finite number of delta functions in a test g_2 will not improve the exponent in (39). This exponent fits the numerical data very well. A best fit of the data in Table II using the functions $d, d^{1/3}, \log_2 d$, appearing in the analysis in the previous section and invoking the existence conjecture of Ref. 7 yields the putative lower bound

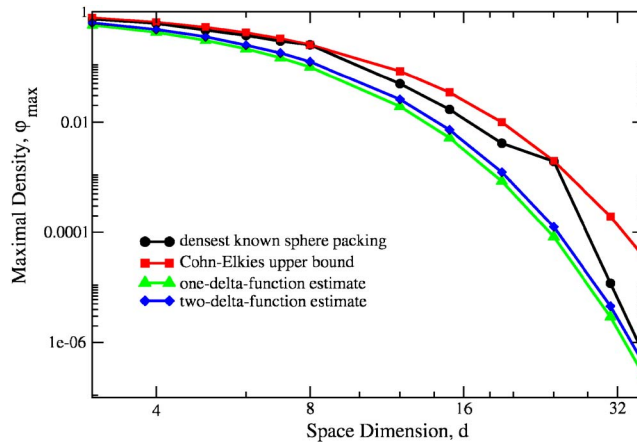


FIG. 4. (Color online) Comparison of different results for the maximal density ϕ_{\max} vs dimension d . From bottom to top: Torquato–Stillinger result (Ref. 7) (1-delta function with gap), one of the results of this paper (2-delta functions with a gap), densest known packings (Ref. 12), and the Cohn–Elkies upper bound (Ref. 4).

$$\phi_{\max} \geq \phi_* \approx 2^{-(0.77865 \dots)d + 2.12(\pm 0.04)d^{1/3} + 0.39(\pm 0.08)\log_2(d) + \dots} \quad (40)$$

The first term is fixed by our analysis; the $d^{1/3}$ term is consistent with the analytic value 2.1247 in Eq. (14). The subleading term $\log_2 d$ in this expression is very difficult to obtain analytically and we have not succeeded in this task. However, it is clear that there is an improvement from the value $\frac{1}{6} = 0.1666 \dots$ appearing in (14). The improvement is also evident from the numbers in Table I.

It is noteworthy that for large d , the optimum gap $\sigma \approx 2.77 \dots / d$ (from a best fit analysis). This scaling with d is slightly different from that found in the previous section and in Ref. 7 (there $\sigma \approx 1.81/d$). The scaling of σ with d , $\sigma \propto 1/d$ is necessary in order not to introduce an exponential suppression of density. In fact, for large d , $(1+c/d)^d \rightarrow e^c$ multiplies the density ϕ in all the formulas (and hence it reduces the terminal value by e^{-c}). A larger gap, say, $\mathcal{O}(d^{-(1-\epsilon)})$, would suppress the density by an exponentially large amount e^{-d^ϵ} .

Table I compares the final results of our analysis for the conjectured lower bound on the maximal density to the previous lower bound, the best known packings, and the optimal upper bound in Ref. 4 for selected dimensions up to $d=150$. As in the previous cases, the Yamada condition³² is violated only for $d=1$. This supports the conclusion reached in Ref. 7 that the Yamada condition appears to only have practical relevance in very low dimensions.

TABLE II. Terminal density ϕ_* for two delta functions and a gap, corresponding optimal gap σ , and optimal average kissing number $Z_{1,*}$ for large d .

d	σ	$Z_{1,*}$	ϕ_*
200	0.013 508	1.57×10^{18}	1.06×10^{-43}
250	0.010 895	7.15×10^{21}	4.18×10^{-55}
300	0.009 132	2.94×10^{25}	1.49×10^{-66}
350	0.007 862	1.12×10^{29}	4.96×10^{-78}
400	0.006 903	2.93×10^{25}	1.56×10^{-89}
450	0.006 154	1.38×10^{36}	4.73×10^{-101}
500	0.005 553	4.67×10^{39}	1.40×10^{-112}

VI. CONCLUSIONS AND OPEN QUESTIONS

The problem of finding the asymptotic behavior of the maximal density ϕ_{\max} of sphere packings in high dimensions is one of the most fascinating and challenging problems in geometry. In this paper, we have shown how using the LP lower bounds and a conjecture concerning the existence of disordered sphere packings based on pair-correlation information, the asymptotic conjectural lower bound⁷

$$\phi_{\max} \geq 2^{-(0.77865\dots)d}, \quad (41)$$

which provides the putative exponential improvement on Minkowski's century-old lower bound (2), is actually much more general than one could have initially surmised. Precisely the same exponential improvement arises for a simpler pair-correlation function than the one employed in Ref. 7 and survives also for a considerable enlargement of the family of test functions g_2 . This family of functions includes two delta functions with a gap [which we have shown improves upon the prefactor multiplying $2^{-(0.77865\dots)d}$ given in Ref. 7] and, we argue, any finite number of delta functions. If this is true, as we believe, it signifies that the *decorrelation principle* alone has a huge predictive power, since an exponential improvement of Minkowski's bound has proved to be an extremely difficult task. We also showed that the asymptotic lower bound on the kissing number, $Z_{\max} \geq 2^{0.22134\dots d}$ (found in Ref. 7) is robust for a large family of test functions.

One outstanding open question is certainly in which sense this is to be interpreted as an asymptotic bound. Based on our present, limited knowledge of optimal sphere packings, we foresee diverse scenarios. In one case, for sufficiently large d , the importance of higher-order correlations is to be neglected altogether and the bound becomes exact by virtue of the *decorrelation principle*. This would mean that the asymptotic Kabatiansky–Levenshtein upper bound is far from optimal: a provocative possibility. In a second scenario, it could be that “special dimensions” continue to exist for which the neglect of higher-order correlations is impossible. In this case, the lower bound obtained by our methods would not apply to these special dimensions but will continue to apply to the other dimensions. On the other hand, if the frequency of appearance of these dimensions over the integers decreases to zero, the decorrelation principle is safe. A third but more pessimistic possibility is that these dimensions are actually becoming more and more frequent, and our conjectural bound would apply only to the subset of remaining dimensions. However, there is absolutely no evidence at present for either the second or third scenario. Our best guess at the moment is that the optimal packings in very high dimensions will possess no symmetry at all and therefore are truly disordered. If so, then the decorrelation principle dictates that pair correlations alone completely characterize the packing in high d , implying that the form of the asymptotic bound (41) is exact!

The fact that pair correlations can completely specify an optimal packing may seem to be counterintuitive, but we can now identify even low dimensions where this phenomenon occurs. Specifically, whenever the LP bounds are exact (i.e., achieve some packing), pair-correlation information is sufficient to determine the optimal packing! This outcome, in all likelihood, occurs in \mathbb{R}^2 , \mathbb{R}^8 , and \mathbb{R}^{24} .^{4,11} This implies that whenever LP bounds are not sharp in low dimensions (albeit without a duality gap³⁷ for any d), information about high-order correlations are required to get optimal solutions.

Another interesting question arises because our procedure, like Minkowski's, is nonconstructive. Specifically, it is an open question whether there exist packing constructions that realize our test g_2 's. If such packings exist, are they collectively or strictly jammed?³⁸ For future investigations, it would be fruitful to determine whether there are periodic or truly disordered packings that have pair-correlation functions that approximate well the ones studied in this paper. If these packings could be identified, one should attempt to ascertain whether the higher-order correlations diminish in importance as $d \rightarrow \infty$ in accordance with the decorrelation principle. If such packings exist (or better, if a d -dependent family of them does), they would enable one to place the putative exponential improvement on Minkowski's bound on a firm, rigorous foundation. We are currently investigating these questions.

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- ¹⁸The density is not necessarily well defined for pathological packings, but in such instances one can take a lim sup of the densities for increasingly large finite spherical regions; see Ref. 17.
- ¹⁹A lattice Λ in \mathbb{R}^d is a subgroup consisting of the integer linear combinations of vectors that constitute a basis for \mathbb{R}^d . A lattice packing P_L is one in which the centers of nonoverlapping spheres are located at the points of Λ . In a lattice packing, the space \mathbb{R}^d can be geometrically divided into identical regions F called *fundamental cells*, each of which contains the center of just one sphere. In the physical sciences, a lattice packing is simply a packings arranged on the sites of a Bravais lattice.
- ²⁰In Ref. 7, a *disordered packing* in \mathbb{R}^d is defined to be a packing in which the pair-correlation function $g_2(\mathbf{r})$ decays to its long-range value of unity faster than $|\mathbf{r}|^{-d-\epsilon}$ for some $\epsilon > 0$. In physical terminology, such a packing will not possess *Bragg peaks*, i.e., possess no-long range order in the infinite-volume limit.
- ²¹Already in \mathbb{R}^{10} , we encounter for the first time a nonlattice (i.e., periodic) packing that is denser than all known lattice packings; see Ref. 12.
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- ²⁴See Ref. 7 and references therein.
- ²⁵G. A. Kabatiansky and V. I. Levenshtein, *Probl. Inf. Transm.* **14**, 1 (1978).
- ²⁶The ghost RSA process is a time-dependent packing in \mathbb{R}^d in which there are no spheres at time $t=0$. For any $t > 0$, sphere placements are attempted by a purely random process and are accepted if they do not overlap any existing sphere in the packing or any *previously* rejected sphere at any previous time. Such spheres are called ghost spheres. In the infinite-time limit, the ghost RSA packings achieve a maximal density of 2^{-d} . See Ref. 6 for more details of this packing and its generalizations.
- ²⁷The well-known standard RSA packing is also a time-dependent packing in \mathbb{R}^d in which there are no spheres at time $t=0$. For any $t > 0$, sphere placements are attempted by a purely random process and are accepted if they do not overlap any current sphere in the packing. In the infinite-time limit, the packing is saturated and its maximal density is achieved.
- ²⁸Based on our knowledge of spin systems in high dimensions, it may be tempting to conclude that the decorrelation principle is an expected “mean-field” behavior, but this cannot be the case for reasons that have already been discussed elsewhere (Refs. 9 and 10).
- ²⁹The structure factor for a generally translationally invariant point process is defined by $S(\mathbf{k}) \equiv 1 + \rho \tilde{h}(\mathbf{k})$, where $\tilde{h}(\mathbf{k})$ is the Fourier transform of the total correlation function $h(\mathbf{r}) = g_2(\mathbf{r}) - 1$ and \mathbf{k} is the wave vector. The structure factor characterizes density fluctuations (variance in the number density) at wave vector \mathbf{k} .
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- ³²M. Yamada, *Prog. Theor. Phys.* **25**, 579 (1961). The Yamada condition is an inequality involving the variance $\sigma^2(\Omega) \equiv \langle (N(\Omega)^2 - \langle N(\Omega) \rangle^2) \rangle$ in the number $N(\Omega)$ of particle centers contained within a region or “window” $\Omega \subset \mathbb{R}^d$, namely, $\sigma^2(\Omega) \geq \theta(1 - \theta)$, where θ is the fractional part of the expected number of points $\rho|\Omega|$ contained in the window. Reference 30 gives explicit representations of the number variance in terms of either the pair-correlation function or the structure factor.
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³⁶LP problems involve the optimization of a linear objective function subject to linear inequality constraints. Every LP problem, referred to as a primal problem, can be converted into a dual problem. If the primal problem is posed as a lower (upper) bound on the objective function, the dual problem is the corresponding upper (lower) bound on the objective function. For further details, the interested reader is referred to R. J. Vanderbei, *Linear Programming: Foundations and Extensions*, 3rd ed. (Springer, New York, 2007).

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