Maximizing the packing density on a class of almost periodic sphere packings

Oliver Knill*

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Abstract

We consider the variational problem of maximizing the packing density on some finite dimensional set of almost periodic sphere packings. We show that the maximal density on this manifold is obtained by periodic packings. Since the density is a continuous, but a nondifferentiable function on this manifold, the variational problem is related to number theoretical questions.

Every sphere packing in $\mathbf{R}^d$ defines a dynamical system with time $\mathbf{R}^d$. If the dynamical system is strictly ergodic, the packing has a well defined density. The packings considered here belong to quasi-periodic dynamical systems, strictly ergodic translations on a compact topological group and are higher dimensional versions of circle sequences in one dimension. In most cases, these packings are quasicrystals because the dynamics has dense point spectrum.

Attached to each quasi-periodic sphere-packing is a periodic or aperiodic Voronoi tiling of $\mathbf{R}^d$ by finitely many types of polytopes. Most of the tilings belonging to the d-dimensional set of packings are aperiodic.

We construct a one-parameter family of dynamically isospectral quasi-periodic sphere packings which have a uniform lower bound on the density when variing the radius of the packing. The simultaneous density bound depends on constants in the theory of simultaneous Diophantine approximation.

1 Introduction

Finding sphere packings in $\mathbf{R}^d$ with maximal density are important mostly unsolved problems with many applications (see [3]). The problem is interesting in geometry, group theory, crystallography or physics. Here, we look at the problem from a dynamical system point of view.

It is still controversial, whether the **Kepler conjecture** claiming that there is no sphere-packing in $\mathbf{R}^3$ with density higher than $\pi/\sqrt{18}$ is open or proven ([8, 11]). Also for dimensions bigger than 3, the best densities are still not known evenso there is a list of candidates (see [2],[3]). According to a general result of Groemer ([6] see also [7]), there exists a sphere packing which has a maximal density.

*Division of Physics, Mathematics and Astronomy, Caltech, Pasadena, CA, 91125, e-mail: *knill@cco.caltech.edu*

Periodic packings and often lattice packings have achieved the highest today known densities (see [3]). Following an advise in [16] p. 188, we restrict us here to a subclass of packings, where we know that the density of the packing exists. This family of quasicrystals, almost periodic sphere-packings in $\mathbf{R}^d$ which form a part of the huge space $\mathcal{S}$ of all packings. Quasicrystalline dense sphere packings are of interest in physics (see for example [14, 1]). The ergodic-theoretical side of the problem comes natural in the context of aperiodic tilings. Tilings and packings are closely related since to every strictly ergodic sphere-packing is attached a tiling of $\mathbf{R}^d$ by Voronoi cells consisting of finitely many types of polytopes.
The quasicrystals in this article are defined by higher dimensional circle sequences and have the property that the densities can be computed explicitely from the parameters. This allows for a machine to search through many of these packings and to determine in each case the exact density. The feature of being able to compute macroscopic quantities like densities for aperiodic configurations was also useful when we studied cellular automata on circle configurations [10]. The main motivation for the present work was to investigate dense packings with a new class of packings. We could consider many packings with high periodicity which are close to the best known packing.

A packing $S \subset \mathbf{Z}^d$ can be described by a configuration $n \mapsto x_n = \{0,1\}^{\mathbf{Z}^d}$. The closure Y of all the translates of x in $\{0,1\}^{\mathbf{Z}^d}$ forms a **subshift** with time $\mathbf{Z}^d$. In general, there exist many shift- invariant measures on Y and the density depends on the choice of the invariant measure. For the packings, we consider here, the subshift Y has a unique shift-invariant measure and it implies that the density is well defined and can explicitly be determined. Moreover, if we make a translation in the $i'th$ coordinate, we get a one-dimensional strictly ergodic subshift for which the dynamical spectrum (and so the diffraction spectrum) is known to be pure point. The packings are therefore crystals or quasicrystals (see [13]).

The organization of this article is as follows. In section 2, we relate sphere packings with dynamical systems and point out, that the uniquely ergodic packings have a well defined density. In section 3, we consider a finite dimensional class of strictly ergodic sphere packings and compute the density of the packings. We show that the density functional takes its maximum on periodic packings. In section 4, we give classes of such packings and relate the problem to find dense packings to number theoretical questions. We also report about packings found by numerical experiments. In section 5, we will construct a one-parameter family of isospectral sphere packings which have a uniform positive density depending on constants in simultaneous Diophantine approximation. In section 6, we discuss a related construction for coverings. Relations with other topics are outlined in section 7 and in section 8, some open problems are summarized.

2 Sphere packings and dynamical systems

A r-**sphere packing** S is a countable set of points in $\mathbf{R}^d$ such that the minimal distance between two points is $\geq 2r$. Let $\mathcal{S}$ be the set of all sphere packings. Define a metric on $\mathcal{S}$ by $d(S,S') = \min(1,\epsilon)$, where ϵ is the smallest number such that $T_x S = S + x = S'$ on the ball $\{||y|| \leq 1/\epsilon\}$ for some $x \in \mathbf{R}^d$. With this metric, which is adapted from the metric for tilings, $(\mathcal{S}, d)$ is a complete metric space. Let $\mathbf{R}^d$ act on $\mathcal{S}$ by translations $T_t(S) = S+t$. Given a specific sphere packing S, we can look at the closure X_S of the orbit $\mathbf{R}^d(S) = \{S+t \mid t \in \mathbf{R}^d\}$. If X_s compact in $\mathcal{S}$, we get a dynamical system $(X_S, \mathbf{R}^d)$, where X_S is a compact metric space on which $\mathbf{R}^d$ acts by homeomorphisms. Such a system is called **minimal** or **almost periodic**, if for every $S \in \mathcal{S}$, the orbit is dense in X_S, it is called **uniquely ergodic**, if there exists exactly one $\mathbf{R}^d$- invariant measure on X_S, **strictly ergodic**, if it is uniquely ergodic and minimal.

Remarks.
1) A metric on $\mathcal{S}$, with respect to which the subset of r-packings in $\mathcal{S}$ becomes compact is described in [5]. For our purposes, the stronger metric d is good enough.
2) In the statistical mechanics literature, a sphere packing is also called a configuration with hard core restriction.
3) By normalization of the distance in $\mathbf{R}^d$, we could assume that a sphere packing has radius $r = 1$. We keep the additional parameter r since we are interested in packings $S \subset \mathbf{Z}^d$.

We call a sphere packing S **rational**, if all points of S belong to a d-dimensional lattice $U \cdot \mathbf{Z}^d \subset \mathbf{R}^d$, where U is an invertible $d \times d$-matrix. On a rational sphere packing, there is a natural $\mathbf{Z}^d$-action, by identifying $\mathbf{Z}^d$ with the maximal subgroup of $\mathbf{R}^d$ which leaves the lattice invariant. The packing S consists then of a subset of the lattice and every rational sphere packing defines so a subshift $\mathcal{Y}_S \subset \{0,1\}^{\mathbf{Z}^d}$. This set $\mathcal{Y}_S$ is is invariant under the $\mathbf{Z}^d$-action. A rational sphere packings is called **strictly ergodic**, if the dynamical system $(\mathcal{Y}_S, \mathbf{Z}^d)$ is strictly ergodic. If every shift of the $\mathbf{Z}^d$-action is periodic, S is called **periodic**,

Remarks.
1) Clearly, a periodic packing is rational and also strictly ergodic.
2) Periodic packings are dense in $\mathcal{S}$ since we can periodically continue a given packing outside a given box. Periodic packings are also dense in the set of rational packings.
3) The name **almost periodic** which stands as a synonym for minimal has no relation with the usual almost periodicity of functions or sequences. The expression almost periodic is however widely used in the topological dynamics and mathematical physics literature.

The lower and upper **densities** of a sphere packing S are defined as

$$\Delta^- = \liminf_{n \to \infty} \frac{|S \cap \Lambda_n|}{|\Lambda_n|} \;, \Delta^+ = \limsup_{n \to \infty} \frac{|S \cap \Lambda_n|}{|\Lambda_n|} \;,$$

where $\Lambda_n = [-n, n]^d$. If $\Delta = \Delta^- = \Delta^+$, then Δ is called the **density** of S.

Lemma 2.1 *For a strictly ergodic sphere packing, the density exists.*

Proof. The limits

$$f \mapsto \phi^{\pm}(f) = \pm \limsup_{n \to \infty} \pm |\Lambda_n|^{-1} \sum_{k \in \Lambda_n} f(T^k(x))$$

define bounded functionals $\phi^{\pm}$ on $C(X)$ which are invariant under the translations $f \mapsto f(T^k)$. By Riesz representation theorem, $\phi^{\pm}(f) = \int f \; d\nu^{\pm}$, where $\nu^{\pm}$ are some measures on X which are invariant under the stricly ergodic $\mathbf{Z}^d$ or $\mathbf{R}^d$ dynamical system (X, T, μ). It follows from the unique ergodicity that $\nu^{\pm} = \mu$ and hence that the two limits coincide. For $\rho : \mathcal{S} \to \mathbf{R}$ given by $\rho(S) = 1_{\{d(S_0, S) < r\}}$ with $S_0 = \{0\} \subset \mathbf{R}^d$, the integral $\int_X \rho \; d\mu$ is the density of the packing. $\square$

Remarks.
1) The above lemma is well known and there are other proofs using more theory. The result follows for example also from a multi-dimensional version of Birkhoff's ergodic theorem (see [4] Chapter VIII). The proof given here uses only lightest tools.
2) There exists a dense set of rational packings in $\mathcal{S}$ which have no density. Proof. Consider a periodic packing S of radius r having density Δ. Take an other periodic packing S' of radius r which has density $\Delta' < \Delta$. Take a first cubic box B_1 centered at zero and fill it with spheres of radius r according to the first packing. Take a second larger cubic box B_2 and fill $B_2 - B_1$ with spheres according to the packing in S'. Make B_2 so large that the density of the packing in this finite box B_2 is smaller than $(\Delta + \Delta')/2$. Take a box B_3 and fill $B_3 - B_2$ with spheres according to α make B_3 so large that the density in the box B_3 is larger than $(2\Delta + \Delta')/3$. Continue inductively so that the finite volume densities are alternatively below $(\Delta + \Delta')/2$ and above $(2\Delta + \Delta')/3$.
Given $\epsilon > 0$, we can make B_1 so large that the distance between the original packing and the modified packing is smaller than ϵ.
3) We are forced to define the packing problem on a subclass of packings since the density is not a continuous function on the set of all packings for which the density exists: take such a packing S and define a sequence of packings S_n obtained from S by deleting all balls in distance less than n from the origin. The packings S_n have all the same density but S_n converges to the $S_\infty = \emptyset$, which is a packing with zero density.

3 Quasi-periodic sphere-packings

We consider now a specific class of almost periodic sphere packings. These packings contain also periodic packings but the computations do not rely on the distinction between periodic and aperiodic. In order to find dense packings experimentally, it was sometimes of advantage, not to distinguish between periodic and aperiodic packings. Take a finite union of disjoint half-open intervals $J \subset \mathbf{R}^1 = \mathbf{R}/\mathbf{Z}$, a rotation vector $\alpha \in \mathbf{R}^d$, a radius $r > 0$ and the standard basis $\{e_i\}_{i=1}^d$ in $\mathbf{R}^d$.

Define $R(r) = \{k \in \mathbf{Z}^d \mid 0 < ||\sum_{i=1}^d k_i e_i||_2 < r\}$, where $||\cdot||$ is the Euclidean l^2-norm in $\mathbf{R}^d$. If $(J + R(r)\alpha) \cap J = \emptyset$, we get for any $\theta \in \mathbf{T}^1$ a sphere-packing

$$S = \{k \in \mathbf{Z}^d \mid \sum_{i=1}^d \theta + k_i\alpha_i \in J\} .$$

If we put a sphere of radius $r/2$ at each point of H, we get a r-packing because the maximal distance between two different points in H is by construction $< r$. This packing is not periodic if one of the numbers α_i is irrational. We call such a packing *quasi-periodic.*

Lemma 3.1 *A quasi-periodic sphere packing is stricly ergodic.*

Proof. Consider the dynamical system $(\mathbf{T}^1, T_i(\theta) = \theta + \alpha_i, dx)$. If all the α_i are rational, then every orbit of this $\mathbf{Z}^d$-action is finite. Every $\theta \in \mathbf{T}^1$ defines a configuration $x_n = 1_J(\theta + n \cdot \alpha)$ and the closure is a finite set in $\{0,1\}^{\mathbf{Z}^d}$ on which the shifts act as permutations. Clearly every orbit is dense and the equal distribution is the only invariant measure. If at least one number α_i is irrational, then every orbit of T is infinite and is dense in $\mathbf{T}^1$. The shift action on the closure X_J of the configuration $x_n = 1_J(\theta + n \cdot \alpha)$ is strictly ergodic since the irrational rotation α_i alone has only one invariant measure μ on X_J and is minimal (see [9] Proposition A.1.). $\square$

Remark.
The density of a quasi-periodic sphere-packing can be approximated explicitely by periodic sphere-packings because every vector α is a limit of rational vectors and the density depends continuously on α. It is not excluded that in some dimension, the highest possible packing is aperiodic, but we will see that if J consists of a single interval, the maximal density is obtained by a periodic packing.

The *center density* δ of a sphere-packing is defined as $\Delta/V(d)$, where Δ is the density and $V(d)$ is the volume of the unit sphere in $\mathbf{R}^d$.

Proposition 3.2 *Assume $(J + R(r)\alpha) \cap J = \emptyset$. The center density of the quasi-periodic or periodic packing is $(r/2)^d|J|$, the density is $V(d)(r/2)^d|J|$.*

Proof. The orbit of a configuration $x_n = 1_J(\theta + n\alpha)$ is a subset of $\{0,1\}^{\mathbf{Z}^d}$ which is shift-invariant. By the above lemma, its closure X is a strictly ergodic set. The density of the configuration $x \in \{0,1\}^{\mathbf{Z}^d}$ is therefore $|J|$ and is independent of $\theta \in J$. The $r/2$-packing $S = \{n \mid x_n = 1\}$ has density $V(d)(r/2)^d|J|$. $\square$

Remark. Note that evenso the map $\alpha \mapsto S(\alpha)$ is not continuous, the density is continuously depending on α.
We can replace the standard basis by any other basis $f_i = Ue_i$ with $U \in GL(d, \mathbf{R})$.

Corollary 3.3 *Given any basis $f_i = Ue_i$ with $U \in GL(d, \mathbf{R})$. Assume $(J + R(r)\alpha) \cap J = \emptyset$ with $R(r) = \{k \in \mathbf{Z}^d \mid ||\sum_{i=1}^d k_i f_i||_2 < r\}$. The density of this packing is $V(d)(r/2)^d|J|/\det(U)$.*

Proof. Every sphere of the packing is in bijective correspondence with a parallelepiped spanned by the basis $f_1, \dots, f_d$, attached to the center of each ball. This parallelepiped has volume $\det(U)$ so that the measure of the sphere divided by $\det(U)$ gives the density in the case when $|J| = 1$. $\square$

Given α, r, we find J consisting of one interval such that $(J + R(r)\alpha) \cap J = \emptyset$. Start with $\theta_0 = 0$ and form the finite set

$$R(r)\alpha = \{\theta_1, \dots, \theta_N\} \subset \mathbf{T}^1 .$$

The points $\theta_1 = c, \theta_N = -c$ nearest to θ_0 are symmetric to 0. Form $J = [0, c)$. We check that $R(r)J \cap J = \emptyset$. The center density of the packing with this interval is then $c(r/2)^d$.

Remarks.
1) We can add a second interval J' as follows. Assume the interval (θ_i, θ_{i+1}) of length l_i is the largest interval disjoint from $R(r) \cdot \alpha$. There are three cases. If $l_i > 2c$, take $J' = [a, b) = [\theta_{i+1} - 2c, \theta_{i+1} - c)$. If $c < l_i < 2c$, define $J' = [a, b) = [\theta_i, \theta_{i+1} - c)$. In the other case, take $J' = \emptyset$. We show now that, $[R(r)\alpha + (J \cup J')] \cap (J \cup J') = \emptyset$. For $\theta \in J$, we have $\theta + R(r)\alpha \notin J$ and $\theta + R(r)\alpha \notin J'$, since J' is disjoint from $J + R(r)\alpha$. For

$\theta \in J'$, we have also that $\theta + R(r)\alpha$ is disjoint from J'. It is also disjoint from J_1, since $R(r)\alpha = -R(r)\alpha$. The center density of the packing is then $(c+b-a)(r/2)^d$.
2) We could proceed as follows to get larger and larger sets J. Given J_n, take any point θ outside $J_n \cup R(r)J_n$. If $R(r)+\theta$ mod 1 is disjoint from J_n, we can find a maximal interval I_θ which has the property $(R+I_\theta)\cap I_\theta = \emptyset$. Form $J_{n+1} = J_n \cup I_\theta$. Repeating this construction leads to a finite or countable union J of half-open intervals which has the property that $(R+J)\cap J = \emptyset$. In other words, we are adding spheres until the covering is saturated, in the sense that there is no longer room with positive density for adding additional spheres. Usually, in our experiments if the first interval is large enough, then J is already saturated and no second interval is needed.
3) For getting high densities, we have to choose r such that the number of lattice points inside the ball of radius r is just below a point of discontinuity. Necessary is $r = \sqrt{n}$, where $n \in \mathbf{N}$ and that there is a lattice point on the boundary of the ball with radius r so that a further increase of r increases the number of lattice points. By a theorem of Lagrange in number theory, this is always true if $d \geq 4$ and $r = \sqrt{n}$. In other words, by extending the variational problem and variing r also, a packing which maximizes the density has the property that r^2 is an integer.
4) We expected to get high densities for radii r, for which many lattice points are on the boundary of a sphere of radius r because of a possible large kissing number. The experiments confirm this in some cases like $r = 5, d = 2, 3$, but it was not the rule.

Proposition 3.4 *There exists a quasi-periodic sphere-packing in $\mathbf{R}^d$ with density*

$$V(d)\frac{r^d}{2^d} \cdot N(d,r,\alpha)$$

where

$$N(d,r,\alpha) = \min_{0<||n||_2<r} |n \cdot \alpha \pmod 1|$$

and where $V(d)$ is the volume of the d-sphere. More generally, given a general basis $f_i = Ue_i$ in $\mathbf{R}^d$. There exists a quasi-periodic sphere packing with density

$$V(d)\frac{r^d}{2^d} \cdot \frac{N_U(d,r,\alpha)}{\det(U)}$$

where $N_U(d,r,\alpha) = \min_{0<||\sum_i n_i U e_i||_2<r} |n \cdot \alpha \pmod 1|$.

Proof. Do the above construction with one interval J of length $N(d,r,\alpha)$ rsp. $N_U(d,r,\alpha)$. □

The next proposition deals with the variational problem to maximize the nondifferentiable function $N(d,r,\alpha)$ over the d dimensional torus of parameters α, when the dimension d and the radius r are fixed. The proposition says that this variational problem has only rational "critical points". It means that on some finite dimensional manifolds of almost periodic packings, the maximal density is achieved by periodic packings.

Proposition 3.5 *The function*

$$\alpha \in \mathbf{T}^d \mapsto N(d,r,\alpha) = \min_{0<||n||_2<r} |n \cdot \alpha \pmod 1|$$

takes its global maximum on a rational point $\alpha \in \mathbf{Q}^d/\mathbf{Z}^d \cap \mathbf{T}^d$. Also all local maxima α are rational.

Proof. Since N is a continuous function on the compact manifold $\mathbf{T}^d$, the maximum is attained. Let β maximize $\alpha \mapsto N(\alpha) = N(d,r,\alpha)$. There exist $n, n' \in \mathbf{Z}$ such that $n'\beta = n\beta \pmod 1$, otherwise $\alpha \mapsto N(\alpha)$ would be strictly monotone and β were not maximal. There exists therefore $m = (m_1, \dots, m_d), k \in \mathbf{N}$ such that $m \cdot \beta = k$. Consider now the $(d-1)$-dimensional surface

$$U^{(1)} = \{\alpha \in \mathbf{T}^d \mid m \cdot \alpha = k\}$$

which contains the maximum. $U^{(1)}$ is topologically a $(d-1)$ dimensional torus. Choose coordinates on $U^{(1)}$ so that α is a $(d-1)$-dimensional vector. Call $\beta^{(1)}$ the maximum β in these coordinates. Again, $\alpha \mapsto N(d,r,\alpha)$ is a linear function on $U^{(1)} \setminus \{\alpha \mid \exists m, k,\ m \cdot \alpha = k\}$ so that the maximum $\beta^{(1)}$ on U_1 satisfies $m^{(1)} \cdot \beta^{(1)} = k^{(1)}$ for some integers $m_1^{(1)}, \dots, m_{d-1}^{(1)}, k^{(1)}$. Define the $(d-2)$-dimensional surface

$$U^{(2)} = \{\alpha \in U^{(1)} \mid m^{(1)} \cdot \alpha = k^{(1)}\}$$

containing the maximum with local coordinates $\beta^{(2)}$.
Inductively, after $d-1$ such steps, we know that the maximum is on a one dimension line $U^{(d-1)}$ which is the intersection of $(d-1)$ rational surfaces projected from $\mathbf{R}^d$ to $\mathbf{T}^d$. Claim: the point on this line, which has maximal distance from 0 has rational coordinates in $\mathbf{T}^d$. Proof. working in the covering of $\mathbf{T}^d$, this claim can be rephrased as follows: given a line segment in $\mathbf{R}^d$ which connects two lattice points $P, Q \in \mathbf{Z}^d$. Any point on this line segment, which maximizes the distance from $\mathbf{Z}^d$ has rational coordinates. This statement is true because the linear projection matrix from $\mathbf{R}^d$ to this line has rational entries (if the basis vector on the line is the vector from P to Q) and therefore every lattice point in $\mathbf{Z}^d$ is mapped onto a rational point.
The same proof works also for local maxima instead of global maxima. $\square$

Remark.
The same argument shows that for any finite set $R \subset \mathbf{Z}^d$ not containing the origin, the function

$$\alpha \in \mathbf{T}^d \mapsto N(d,r,\alpha) = \min_{n \in R} |n \cdot \alpha \pmod 1|$$

takes its global maximum on a rational point $\mathbf{Q}^d/\mathbf{Z}^d \cap \mathbf{T}^d$. We can consider therefore any packing problem, where the spheres are replaced by some compact set $K \subset \mathbf{R}^d$. The analogue problem is to find for a given r, the densest packing of $\mathbf{R}^d$ with copies $n + rK, n \in \mathbf{Z}^d$ of $r \cdot K$. The same construction gives a d-dimensional manifold of almost periodic packings for which the density exists. The maximal density on this manifold is obtained by periodic packings.

4 Examples of quasi-periodic packings

Lattice packings. Assume the packing is a lattice packing defined by the generator matrix U. We can take $r = 1$ so that $R(1) = \emptyset$ and $J = \mathbf{T}^1$ leading to $N(d,1,\alpha) = 1$ independent of α. The density of the lattice packing is $V(d)/(2^d \det(U))$. For example, for $d = 2$ and with the generator matrix

$$U = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix} ,$$

the density is

$$V(2)\frac{1}{2^2}\frac{N(2,1,\alpha)}{\det(U)} = \pi/\sqrt{12}$$

which is known to be the highest density in two dimensions.

Packings with radius $r = \sqrt{2}$ give the lattices D_d. Take $r = \sqrt{2}$ and the standard basis e_i. We have

$$R(\sqrt{2}) = \{(\pm 1, \dots, 0, 0), (0, \pm 1, \dots, 0), \dots, (0, 0, \dots, \pm 1)\} .$$

With $\alpha = (1, 1, \dots, 1)/2$ and $J = [0, 1/2]$, we get $N(3, \sqrt{2}, \alpha) = 1/2$ and the density is $V(d)/2^{d/2+1}$ corresponding to a center density $2^{-(d/2+1)}$. These packings are lattice packings called D_d. In dimensions $d = 3, 4, 5$, these packings are the packings with the highest known density like for $d = 3$, the density is $V(3)\sqrt{2}^3/2^3 N(2,1,\alpha) = \frac{4}{3}\pi \cdot 1/(4\sqrt{2})$ and in four dimensions $V(4)\sqrt{2}^4/2^4 N(2,1,\alpha) = \pi^2/2 \cdot 1/8$.

Packings with radius $r = \sqrt{3}$. With $r = \sqrt{3}$, and $\alpha = (1, 2, 3, \dots, d)/2d$, we get $N(d, \sqrt{3}, \alpha) = 1/(2d)$ and a center density $(\sqrt{3}/2)^d/(2d)$. This density is larger than the density of D_d for $d > 12$. These packings were the densest we found numerically for $d = 2, 3, 4, 5$ in the class of quasi-periodic packings with $r = \sqrt{3}$.

Packings with radius $r = 2$. We have the problem to find integers p and $a_1, \dots a_d$ such that in the group $\mathbf{Z}_p$, no sum $\sum n_i^2 a_i$ gives zero if $\sum_i n_i^2 < r$. In other words, all sums $a_{i_1} \pm a_{i_2} \pm a_{i_3}$ are different from zero modulo p. We can build solutions by defining recursively a sequence a_n with the linear difference equation $a_1 = 1, a_2 = 2$, $a_n = a_{n-1} + a_{n-2} + 1$ and define the vector $\alpha = (a_1, a_2, \dots, a_d)/(2a_d)$. In the case $d = 2, \alpha = (1,2)/4$ or $d = 3, \alpha = (1, 2, 4)/8$, or $d = 4, \alpha = (1, 2, 4, 7)/14$, these were the densest 2-packings we found in our class. For $d = 5$, the 2-packing $\alpha = (1, 3, 5, 7, 9)/18$ was denser than the 2-packing determined by $\alpha = (1, 2, 4, 7, 12)/24$.

This construction of families of packings with increasing dimension can be generalized for any r. The problem is to find the smallest $p = p(d, r)$, such that there exist d numbers $a_1, \dots, a_d \in \mathbf{Z}_p$ such that for any $n \in \mathbf{Z}^d$ with $||n||_2 < r$, the equation $n \cdot a = 0$ in $\mathbf{Z}_p$ has no solution. The center density of the corresponding packing is then $(r/2)^d/p(d, r)$. We rephrase the result in the following proposition.

Proposition 4.1 *Fix the dimension d and the radius r. If we can find d numbers $a_1, \dots, a_d$ in the group $\mathbf{Z}_p = \mathbf{Z}/(p\mathbf{Z})$ such that for any $n \in \mathbf{Z}^d$ with $0 < n_1^2 + \ldots + n_d^2 < r^2$, the equation*

$$n \cdot a = 0 \bmod p$$

has no solution, then there exists a rational r-packing $S \subset \mathbf{Z}^d$ with density $V(d)(r/2)^d/p$.

Proof. We do the construction with the vector $\alpha = (a_1, \dots, a_d)/p$ and the interval $J = [0, 1/p)$. Given a point $\theta \in J$ and n with $||n||_1 < r$, then $\theta + n \cdot \alpha$ is not in J. $\square$

Remark.
For prime p, a packing in the proposition defines a code in the vector space $\mathbf{Z}_p^d$. In coding

theory, one considers however rather the packing problem with the Hamming metric instead of the Eucledean metric.

We found some good packings in the special case, when r is an integer and $a_1 = 1, a_2 = r, a_3 = r^2, \dots, a_d = r^{d-1}$.

Corollary 4.2 *Let r be an integer and let p be the smallest integer such that*

$$n_1 + n_2 r + n_3 r^2 + \dots + r_d r^{d-1} = 0 \bmod p$$

has no solution for $0 < \sum_{i=1}^{d} n_i^2 < r$. Then there exists a sphere packing with density $V(d)(r/2)^d/p$.

Remarks.
1) Because of the periodicity of the packing, we have for even r that $p - r/2$ is a multiple of r and that for odd r, $p - (r+1)/2$ is a multiple of r.
Example: for $r = 89$, $p = 502984 = (r+1)/2 + 5651 \cdot r$, this gives a packing with density 0.73386212.
2) The construction can be modified by taking for example $\alpha = (1, r+1, r(r+1))/p'$ with suitable p', which gives for some r denser packings than $\alpha = (1, r, r^2)/p$.

We were also looking for dense packings using a multiscale Monte Carlo method. We restricted ourselves to the standard basis in $\mathbf{R}^d$ and to packings defined by one interval and went only up to dimension 5. One method was to shoot randomly vectors α for fixed r and to adapt the search step near good parameters. We did not assume that the best density is obtained for a rational α. Indeed, we conjectured and proved only after having done some experiments that the maxima are rational. For larger values of r and especially for higher dimensions, the searches need a lot of computing time. The reason is that for fixed r and d, the function $\alpha \mapsto N(d, r, \alpha)$ is a piecewise linear function having gradients of the order r^d. We would need therefore to check roughly at $(r^d)^d$ points in order to find the global maximum since so many local maxima are expected. This is an very time consuming task also for quite small r and d's. The huge number of local minima is also the reason why the common methods for minimizing multidimensional functions like the downhill simplex method would not work well here. The function $\alpha \mapsto N(d, r, \alpha)$ is just too wiggly.

Some good packings were obtained by taking a good solution $(d, r, (\alpha_1, \dots, \alpha_d))$ and choosing α_{d+1} so that the packing $(d+1, r, (\alpha_1, \dots, \alpha_{d+1}))$ has maximal density. This is motivated (evenso there is no direct relation) by the laminated lattice construction (see [3]), which also constructs d-dimensional packings by building up layers of $(d-1)$-dimensional packings which are known to be dense.

We never found a denser packing while using two intervals. The search is also algorithmically more expensive, since we have to order the set $R(r) \cdot \alpha$ (mod 1).

r	α	density
$\sqrt{2}$	$(1,1,1)/2$	0.740480
3	$(2,5,6)/20$	0.706858
$\sqrt{13}$	$(8,17,23)/35$	0.701206
5	$(19,5,37)/91$	0.719229
7	$(21,150,194)/252$	0.712676
12	$(60,630,783)/1270$	0.712424
31	$(1,31,961)/21623$	0.721386
38	$(1,38,1444)/39729$	0.723172
65	$(1,65,4225)/196463$	0.731910
89	$(1,89,7921)/502984$	0.733862
120	$(1,120,14400)/1231260$	0.734830

Table 1. Some examples of packings in three dimension. The packing with radius $\sqrt{2}$ is the Kepler packing. The packing with radius 120 gives a slightly denser packing as the packing reported in [17] using Penrose tilings which have densities accumulating by 0.7341.

r	α	density
$\sqrt{2}$	$(1,1,1,1)/2$	0.616850
$\sqrt{3}$	$(1,2,3,4)/8$	0.346978
2	$(2,7,10,13)/14$	0.352486
3	$(48,275,395,419)/435$	0.459447
4	$(81,105,139,169)/185$	0.426794
5	$(20,76,148,167)/364$	0.529557
19	$(1,19,19^2,19^3)/72020$	0.558099

Table 2. Some examples of packings in four dimension. The first packing is the packing which is believed to be the densest.

r	α	density
$\sqrt{2}$	$(1,1,1,1,1)/2$	0.465260
$\sqrt{3}$	$(1,2,3,4,5)/10$	0.256420
2	$(3,9,11,13,17)/18$	0.292433
$\sqrt{5}$	$(1,2,4,8,15)/31$	0.296628
3	$(2165,1835,1154,1575,499)/2178$	0.238570
5	$(80,304,592,668,687)/1456$	0.353051

Table 3. Some examples of packings in five dimension. The first packing is the packing which is believed to be the densest.

5 Isospectral packings with a simultaneous density bound

If we allow to vary r but fix the dynamical system of the packing, the construction of packings with simultaneous lower density bound has a relation with simultaneous Diophantine approximation.

A vector $\alpha = (\alpha_1, \dots, \alpha_d)$ is called *badly approximable by rational numbers* if there exists a constant C such that for all $n \in \mathbf{Z}^d$ and $p \in \mathbf{Z}$

$$|n \cdot \alpha - p| \geq C \cdot ||n||_1^{-d} ,$$

where $||n||_1 = \sum_{i=1}^d |n_i|$. Such numbers exist (see Theorem 6F in [12]). Denote with $C(d)$ the maximum of all possible constants C.

Proposition 5.1 *There exists a one-parameter family S_r of dynamically isospectral quasi-periodic sphere-packings in $\mathbf{R}^d$ with spheres of radius r and $S_r \subset \mathbf{Z}^d$ such that the center density is bounded below by $C(d)2^{-d}d^{-d/2}$, independent of r.*

Proof. We show that there exists $\alpha \in \mathbf{T}^d$, such that $N(d, r\alpha) \geq C(d) \cdot r^{-d} d^{-d/2}$ for all r. By Hölder's inequality, $||n||_1 \leq ||n||_2 ||1||_2 = ||n||_2 \sqrt{d}$. We get therefore for such α

$$|n \cdot \alpha - p| \geq C(d) \cdot d^{-d/2} ||n||_2^{-d}$$

for all $n \in \mathbf{Z}^d$ and $p \in \mathbf{Z}$. This means that

$$|n \cdot \alpha| \mod 1 \geq C(d) \cdot d^{-d/2} r^{-d}$$

for all $||n||_2 \leq r$.
The subshift $X \subset \{0,1\}^{\mathbf{Z}^d}$ obtained by closing the set of translates of $x_n = 1_J(\theta + n\alpha)$ in the product topology is strictly ergodic and the shift T_i on X is measure theoretically isomorphic to a factor of $\theta \mapsto \theta + \alpha_i$. If the set J is an interval of length less than $1/2$, the shift T_i is measure theoretically isomorphic to $\theta \mapsto \theta + \alpha_i$ and has the point spectrum $\{e^{2\pi i k \alpha_i} \mid k \in \mathbf{Z}\}$. The spectrum of the packing is therefore $\{e^{2\pi i k \alpha_i} \mid k \in \mathbf{Z}, 1 \leq i \leq d\}$. $\square$

Remark.
It is trivial to get in any dimension packings with a center-density higher than $C(d)2^{-d}d^{-d/2}$ because $C(d) \leq 1$. The uniform bound for the density in r gives not dense packings and the nontriviality of Proposition 5.1 lies in the fact that the packings are dynamically isospectral in the sense that they have the same dynamical point spectrum and that we can do the packing simultaneous for any $r > 0$. The estimate $N(d, r\alpha) \geq C(d) \cdot r^{-d} d^{-d/2}$ is crude for small r.

6 Coverings

The algorithm to compute packings can be modified to get coverings. Assume, we have an interval $J \subset \mathbf{T}^1$ such that $R(r)J = \mathbf{T}^1$. In this case, the spheres with centers in

$$S(\theta) = \{k \in \mathbf{Z}^d \mid \sum_{i=1}^d \theta + k_i \alpha_i \in J\}$$

and radius r are covering all $\mathbf{Z}^d$ and the spheres of radius $r + \sqrt{d}/2$ are covering the whole space $\mathbf{R}^d$. The density of the covering is

$$V(d)|J|(r + \sqrt{d}/2)^d .$$

Proposition 6.1 *There exist sphere-coverings of $\mathbf{R}^d$ with densities*

$$V(d)(r+\sqrt{d}/2)^d \cdot M(d,r,\alpha) \ ,$$

where

$$M(d,r,\alpha) = \max_{||n||_2 \leq r} \ \min_{||m||_2 \leq r, m \neq n} |(n-m)\alpha \pmod 1| > 0 \ .$$

Proof. Given parameters d, r and α, we can find $M(d,r,\alpha)$ such that $(n-m)\alpha \mod 1 \geq M(d,r,\alpha)$ for all $||n||_2, ||m||_2 \leq r$ satisfying $n\alpha \neq m\alpha \pmod 1$. We can choose for the interval J the largest gap in the finite set $R(r)\cdot\alpha \subset \mathbf{T}^1$, since then, $R(r)J$ is a covering of $\mathbf{T}^1$. The length of J is $M(d,r,\alpha)$. $\square$

Remark.
This proposition implies that in order to get a good covering, the parameters r and α have to be chosen in such a way that $R(r)\cdot\alpha \subset \mathbf{T}^1$ is as homogeneous as possible. The computations for coverings are more involved as the computations for packings since the determination of the set $R(r)\cdot\alpha$ mod 1 includes a time-consuming sorting.

7 Related topics

Crystallographic considerations. The packing question for spheres has been formulated by Hilbert for general compact subsets K of $\mathbf{R}^d$. An example is to replace the Eucledean norm by the l^p norm $||n||_p = (\sum_{i=1}^d |n_i|^p)^{1/p}$ and to pack $\mathbf{R}^d$ with with l^p spheres and clearly for $p=1$ or $p=\infty$, the maximal packing density is 1 and different p will probably lead to different lattices with optimal density. Parameters p, where the optimal packing type changes should be considered as a bifurcation parameter.
For general K, the construction of quasiperiodic packings is the same as already described. We have only to replace $||n||_2 < r$ by $n \in \mathrm{int}(K)$ to obtain the corresponding densities. General packing problems with different type of subsets K are interesting and relevant in crystallography or chemistry, where K takes the shape of a molecule. The same proof as shown above shows that the maximal packing density on d-dimensional manifolds of quasi-periodic packings is attained by periodic packings if we take only copies of K which are obtained from K by translation by $n \in \mathbf{Z}^d$. Removing the last restriction might lead in general to aperiodic packings with maximal density: an indication is that there exist convex sets in $\mathbf{R}^3$, the Schmitt-Conway-Danzer tiles, for which the densest packing is aperiodic with density 1. We mention also a result in [15] which says that for a generic set of convex sets in the plane, the densests packing is not lattice like.

Quasicrystals. Crystals in nature are often periodic. A situation closest to the periodic case are quasi-periodic crystals which are a family of so called quasicrystals. Our result that in a class of quasi-periodic crystals, the maximal density is attained on periodic crystals can have physical relevance since high densities are favored by stable crystalline structures.

Defects. If the packing is almost periodic, there are large domains, where the packing looks periodic, but there must be defects, if the lattice is not periodic. For $\epsilon > 0$, consider the ϵ-collar K_ϵ of the packing S which consists of all points in $\mathbf{R}^d$ which have distance $\leq \epsilon$ from any ball. There exists a largest $\epsilon > 0$, such that the complement of K_ϵ still percolates. The defect, the complement of K_ϵ with critical ϵ is not necessarily almost periodic since the topology of K_ϵ does not depend continuously on ϵ.

Minimizing energy. Moving on the manifold of almost periodic rational r-packings parametrized by $\alpha \in \mathbf{T}^d$ corresponds to (non continuous) deformations of the crystal. The density, when considered as a negative "energy" of the crystal is a piecewise linear continuous function on the parameters. Variational methods do not apply in order to find the maximal density which correspond to minimizing the energy because the energy is not differentiable at the maximum. However, we have seen that the minimal energy on this manifold is obtained by periodic crystals. Since atomic dense packings are believed to be fundamental in condenced matter, our toy model can in principle explain an aspect of the stability of crystals. Moreover, the periodicity of some of the crystals can be so large that it would be hard to distinguish them experimentally from a true quasicrystal.

Aperiodic Voronoi tilings. For strictly ergodic packings, there exists a constant C such that if $x_n = 1$ then there exists $x_m = 1$ with some m satisfying $||m - n||_2 < C$. In other words, there are only finitely many sphere-configurations which can occur in a ball of given radius. The Voronoi tiling of $\mathbf{R}^d$ is built up by finitely many Voronoi simplices. This Voronoi decomposition is an **aperiodic tiling** of $\mathbf{R}^n$ if α rationally independent.

Diffraction spectrum. The diffraction spectrum of the quasicrystals considered here can be computed explicitely: it is a point measure with weights given by a Fourier transform of 1_J (see [10]).

Random sphere packings. We should compare the quasi-periodic packings in $\mathbf{R}^3$ with random sphere packings, which are interesting from the practical point of view. In three dimensions, computer simulations and experiments with large containers of steel balls give a density of 0.6366 (see [18]). Higher densities are no more believed to be random, since the high density is then obtained by crystalisation. Almost periodic sphere packings in three dimensions with higher densities are obtained for most radii r.

Generalization of the construction. The construction could be generalized in the following way. Take any compact abelian group G (generalizing $G = \mathbf{T}^1$) and d commuting group translations $T_1, \dots T_d$. Consider a ring $\mathcal{J}$ of measurable sets (generalizing the ring of half open intervals), where each element in $\mathcal{J}$ different from has positive Haar measure and such that the boundary of every $J \in \mathcal{J}$ has zero Haar measure.

Take $J \in \mathcal{J}$ with maximal measure such that $[J + R(J,r)\alpha] \cap J = \emptyset$ and do the same construction as before. We get a strictly ergodic subshift defining the centers of a sphere packing with spheres of radius $r/2$ and the packings define quasicrystals with pure point dynamical spectrum and so pure point diffraction spectrum. We think however that no other group is as convenient as $G = \mathbf{T}^1$. Taking the p-adic group would be a natural choice from the dynamical systems point of view.

A replacement of the irrational rotation with d commuting homeomorphisms of the circle does not lead to more general packings: if one of the rotation numbers of these homeomorphisms is irrational, then this $\mathbf{Z}^d$- action is topologically conjugated to the action given by the irrational rotations. The subtle and still unsolved problem, whether d commuting circle diffeomorphisms are smoothly conjugated to irrational rotations is not involved.

8 Questions

A number theoretical question is: what is the maximal density of a quasi-periodic sphere packing in $\mathbf{R}^d$ with spheres of radius r centered on a subset of $\mathbf{Z}^d$.

Related (but not equivalent) to this question is the problem to find

$$\max_{\alpha \in \mathbf{T}^d} \min_{0<||n||_2<r} |n \cdot \alpha \pmod 1|$$

in dependence of r. We know that the maximum is always taken for rational α.
This leads to the number theoretical problem to find for fixed $r > 0$, the smallest cyclic group $\mathbf{Z}_p = \mathbf{Z}/(p\mathbf{Z})$ such that there exist $a_1, \dots, a_d \in \mathbf{Z}_p$ such that for any $n \in \mathbf{Z}^d$ with $0 < n_1^2 + \dots + n_d^2 < r^2$, the equation

$$\sum_{i=1}^{d} n_i \cdot a_i = 0 \bmod p$$

has no solution in $\mathbf{Z}_p$.

We also do not know if we can in all dimensions get close to the highest densities by choosing a special sequence of α's. In dimensions up to 6, a class of dense packings can be obtained by $\alpha = (1, r, r^2, \dots, r^{d-1})/p$ with odd r and $p = p(r,d) = (r+1)/2 + qr$ is the smallest integer, such that the density is not vanishing. The densities were converging to the highest known densities for $r \to \infty$.

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