The covering problem related to quasicrystals

Ľubomíra Balková, Zuzana Masáková

Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Trojanova 13, 120 00 Praha 2, Czech Republic

We study mathematical models of quasicrystalline materials — non-crystallographic solids with long range aperiodic order. A natural generalization of crystallographic lattices are the so-called Meyer sets. They are uniformly discrete, relatively dense point sets $\Sigma \subset \mathbb{R}^n$ with the property of almost lattices: $\Sigma - \Sigma \subset \Sigma + F$ for F finite. This property ensures that there is only a finite number of local configurations of atoms in the model of the material. The most commonly studied class of Meyer sets arises in the well known cut-and-project scheme. For cut-and-project sets $\Sigma(\Omega)$ with compact acceptance window $\Omega \subset \mathbb{R}^d$ we study a finite set F of the Meyer property. This task can be transformed into the problem of covering of the difference set $\Omega - \Omega$ by open copies Ω°. The cardinality $f(\Omega)$ of the minimal covering is called the Meyer number of Ω. We show that f is bounded on the space of convex compact sets $\Omega \subset \mathbb{R}^d$. We give estimates on the universal upper bound of the Meyer number of $\Omega \subset \mathbb{R}^2$ and $\Omega \subset \mathbb{R}^3$. We determine the values $f(\Omega)$ for some special types of $\Omega \subset \mathbb{R}^2$. We further show that f is not bounded if we relax the condition of convexity.

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1 Introduction

The fundamental 'law' of crystallography says that a crystal cannot have icosahedral symmetry. However, in 1984 Schechtman announced existence of materials, whose diffraction diagrams showed bright points organized into 10–, 6– and 2–fold symmetry. This corresponds exactly to icosahedron which has 5–, 3–, and 2–fold axes. In present days, crystallographers know materials whose diffraction images have also other crystallographically forbidden symmetries, namely 8– and 12–fold symmetry. Since the accuracy of experimental instruments is finite, the diffraction images reveal a discrete diagram, although they are in fact densely covered by diffraction marks. Such materials are said to have 'essentially discrete diffraction diagram'. In order to obtain such a diffraction image, the material must have a certain long–range order, although the microscopic structure is not a lattice. A big progress in mathematical modelling of these materials, called 'quasicrystals', in recent years is due to J. Lagarias, M. Baake, R.V. Moody, and many others. For a general overview on the mathematical theory see [1].

In a mathematical model of a solid state material we represent position of atoms as points in the space. The model is ideal, i.e. infinite. The requirement that the points should 'uniformly' fill the entire space is characterized by the so-called Delone property:

Definition 1.1. A set $\Lambda \subset \mathbb{R}^d$ is Delone, if there exist $r_1, r_2 > 0$ such that
(i) Λ is *uniformly discrete*: $\|x - y\| \geq r_1$ for any $x, y \in \Lambda$, $x \neq y$.

(ii) Λ is *relatively dense*: $B(x, r_2) \cap \Lambda \neq \emptyset$ for any $x \in \mathbb{R}^d$, where $B(x, r_2)$ is the d–dimensional ball of radius r_2 centered at x.

A suitable model satisfying the above property are the point sets arising in the so-called cut-and-project scheme. Roughly speaking, the set arises as a projection of chosen points of a higher–dimensional lattice on a lower–dimensional 'physical space'. The choice of lattice points is controlled by an 'acceptance window' in the non-physical 'inner space'. The definition of cut-and-project sets which is provided below is not the most general one (for that see [4, 5]). In our considerations both physical and inner spaces are Euclidean. Patera in [6] shows how to choose the lattice and the projection, in order to obtain quasicrystal models with 5–fold symmetries, which have been observed in nature [7].

Definition 1.2. Let V_1 and V_2 be non-trivial subspaces of $\mathbb{R}^n$ such that $V_1 \oplus V_2 = \mathbb{R}^n$, the restriction of π_1 on the lattice $\mathbb{Z}^n$ is one-to-one, and $\pi_2(\mathbb{Z}^n)$ is dense in V_2, where π_1, π_2 are the projections on V_1 along V_2, and V_2 along V_1, respectively. Let Ω be a compact set with non-empty interior Ω°. The set

$$\Sigma(\Omega) := \{\pi_1(x) \mid x \in \mathbb{Z}^n \, , \, \pi_2(x) \in \Omega\}$$

is called a cut-and-project set with acceptance window Ω.

2 Cut-and-project sets and the Meyer number

It has been shown [4] that every cut-and-project set satisfies the Meyer property, i.e. is Delone and

$$\Sigma(\Omega) - \Sigma(\Omega) \subset \Sigma(\Omega) + F \tag{1}$$

for some finite set F. Obviously, $F \subset \pi_1(\mathbb{Z}^n)$ and for the finite set $G := \pi_2\pi_1^{-1}(F)$ we have

$$\Omega - \Omega \subset \Omega + G \, . \tag{2}$$

The converse is however not that simple. Having $G \subset V_2$ which satisfies (2), it is not always possible to find F of the same cardinality, so that (1) holds, which comes from the fact that G may not be a subset of $\pi_2(\mathbb{Z}^n)$. However, this inconvenience can be avoided if we study covering of the difference set $\Omega - \Omega$ by copies of the interior Ω°, namely

$$\overline{\Omega - \Omega} \subset \Omega^\circ + G \, . \tag{3}$$

Having such G and due to the fact that $\pi_2(\mathbb{Z}^n)$ is dense in V_2, we can clearly find a set $\tilde{G} \subset \pi_2(\mathbb{Z}^n)$ of the same cardinality as G and satisfying (2). Therefore we may set $F = \pi_1\pi_2^{-1}(\tilde{G})$ to obtain (1) with $|F| = |G|$.

The main point of interest of this paper can thus be formulated as follows: For compact sets $\Omega \subset \mathbb{R}^d$ with non-empty interior we are interested in the cardinality of the minimal finite set G satisfying (3). This cardinality is denoted by $f(\Omega)$ and called the *Meyer number* of Ω. Formally,

$$f(\Omega) := \min\{k \in \mathbb{N} \mid \exists\, G \subset \mathbb{R}^d \, , \text{ satisfying } \overline{\Omega - \Omega} \subset \Omega^\circ + G \text{ and } |G| = k\} \, .$$

Thus the study of the Meyer property of cut-and-project sets is transformed into a covering problem of convex sets. We want to determine or estimate the Meyer number for compact convex sets $\Omega \subset \mathbb{R}^d$ with non-empty interior. In what follows we state the results about the Meyer number obtained in [2], in particular the fact that on the space of all convex acceptance windows Ω the Meyer number is bounded and if we relax the condition of convexity, such statement is no longer true. We further provide estimates on the universal upper bound on the Meyer number in dimension two and in dimension three.

3 Boundedness of the Meyer number

The most important result about the Meyer number is formulated as follows.

Theorem 3.1. *For every dimension $d \in \mathbb{N}$, there exists a constant $K_d \in \mathbb{N}$, such that for all convex compact sets $\Omega \subset \mathbb{R}^d$ with non-empty interior we have $f(\Omega) \leq K_d$. Moreover, K_d is smaller or equal to the number of d-dimensional unit balls needed for covering $\overline{B(0,2d)} \subset \mathbb{R}^d$.*

The proof of Theorem 3.1 can be found in a detailed form in [2]. Here we provide a sketch which allows us to determine also the estimates on the Meyer number. Crucial for the proof of Theorem 3.1 is the following assertion taken from [3].

Theorem 3.2 (John). *For every convex compact set Ω with non-empty interior in $\mathbb{R}^d$ there exists a closed ellipsoid E such that $E+z \subset \Omega \subset dE+z$, where $z \in \mathbb{R}^d$.*

Proof of Theorem 3.1. Using Theorem 3.2 there exists a closed ellipsoid $E \subset \mathbb{R}^d$ such that $E+z \subset \Omega \subset dE+z$. We find a non-singular affine map A such that $A(E+z) = \overline{B(0,1)}$ and $A(dE+z) = \overline{B(0,d)}$. Then $B(0,1) \subset (A\Omega)^\circ \subset B(0,d)$. Since $\overline{B(0,2d)}$ is compact, the number of copies of $B(0,1)$ needed to cover it is finite, say n. We have thus

$$\overline{B(0,2d)} \subset \big(x_1 + B(0,1)\big) \cup \cdots \cup \big(x_n + B(0,1)\big)\,,$$

for some $x_1, \ldots, x_n \in \mathbb{R}^d$, then

$$A\Omega - A\Omega \subset \overline{B(0,d) - B(0,d)} = \overline{B(0,2d)} \subset \big(x_1 + B(0,1)\big) \cup \cdots \cup \big(x_n + B(0,1)\big) \subset \\ \subset \big(x_1 + (A\Omega)^\circ\big) \cup \cdots \cup \big(x_n + (A\Omega)^\circ\big)\,.$$

It is not difficult to show that the function f is invariant under affine transformations of Ω. More precisely, if $A : \mathbb{R}^d \to \mathbb{R}^d$ is a bijective affine map, then $f(A\Omega) = f(\Omega)$ for every convex compact set $\Omega \subset \mathbb{R}^d$ with non-empty interior. Therefore the above inclusion implies $f(\Omega) = f(A\Omega) \leq n$, what was to show. □

4 Unboundedness of f on the space of general compact sets

Sofar we have treated only convex compact sets in $\mathbb{R}^d$. We stand in front of a natural question. Is the function f bounded even if we relax the condition of convexity? The answer is negative.

Proposition 4.1. *There exists a sequence* $(\Omega_n)_{n\in\mathbb{N}}$ *of compact sets in* R^d *with non-empty interior, such that* $\lim_{n\to\infty} f(\Omega_n) = +\infty$.

Proof. We construct the counterexample of boundedness of the function f in dimension 2. Generalization to higher dimensions is straightforward. Let Ω_n be compact sets with non-empty interior containing the line segments $\{(t,0) \mid t \in [-1,1]\}$, $\{(0,t) \mid t \in [-1,1]\}$ for all $n \in \mathbb{N}$, and such that $\lim_{n\to\infty} \mathrm{vol}(\Omega_n) = 0$.

Then obviously $\Omega_n - \Omega_n$ contains the square of side length 1 centered at the origin, $\{(t_1,t_2) \mid t_1,t_2 \in [-1,1]\}$. For the volume of $\Omega_n - \Omega_n$ we thus have $\mathrm{vol}(\Omega_n - \Omega_n) \geq 4$. Therefore

$$f(\Omega_n) \geq \frac{\mathrm{vol}(\Omega_n - \Omega_n)}{\mathrm{vol}(\Omega_n)} \geq \frac{4}{\mathrm{vol}(\Omega_n)},$$

which implies $\lim_{n\to\infty} f(\Omega_n) = +\infty$, what we wanted to show. □

Let us mention that we can construct the counterexample even on the sets which are the nearest generalization of convex sets, namely star–shaped sets. (We say that $\Omega \subset \mathbb{R}^d$ is star–shaped, if there exists an $x \in \mathbb{R}^d$ such that $\lambda x + (1-\lambda)y \in \Omega$ for every $y \in \Omega$ and all $\lambda \in (0,1)$.) An example of a sequence of star–shaped sets Ω_n satisfying $\lim_{n\to\infty} f(\Omega_n) = +\infty$ and the corresponding difference sets $\Omega_n - \Omega_n$ can be found in Figure 1.

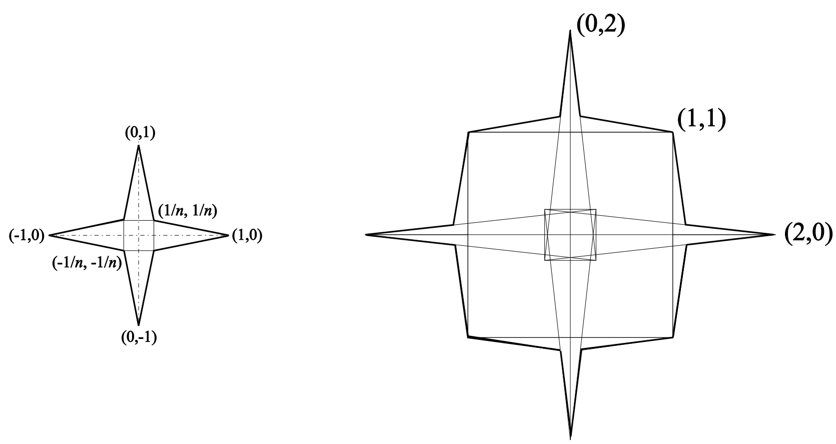

Fig. 1. Illustration of a sequence of star–shaped sets Ω_n, $n \in \mathbb{N}$, satisfying $\lim\limits_{n\to\infty} f(\Omega_n) = +\infty$. The left hand part of the figure shows Ω_n, on the right hand side there is $\Omega_n - \Omega_n$.

Note also that we have omitted the proof of unboundedness of f in dimension one. There every star–shaped set is convex, the counterexample in $\mathbb{R}$ must therefore be built on non-connected sets. The construction of such a sequence of sets is simple but rather technical.

5 Universal bound on the Meyer number for convex sets in $\mathbb{R}^2$

In this section we provide an estimate on the value of the function f for two–dimensional convex compact sets Ω, i.e. on the constant K_d of Theorem 3.1 for $d = 2$. According to the theorem, the universal bound K_2 on the Meyer number of convex sets in $\mathbb{R}^2$ is smaller or equal to the number of copies of the open 2-dimensional unit ball $B(0,1)$ needed to cover the closed ball $\overline{B(0,4)}$. The result is stated in the following proposition.

Proposition 5.1. *Let Ω be a convex compact set in $\mathbb{R}^2$. Then $f(\Omega) \leq K_2 \leq 26$.*

Proof. Figure 2 shows that it is possible to cover $\overline{B(0,4)}$ by 26 translated copies of the ball $B(0,1)$. Hence, $f(\Omega) \leq 26$ for every convex compact set Ω with non-empty interior in $\mathbb{R}^2$. □

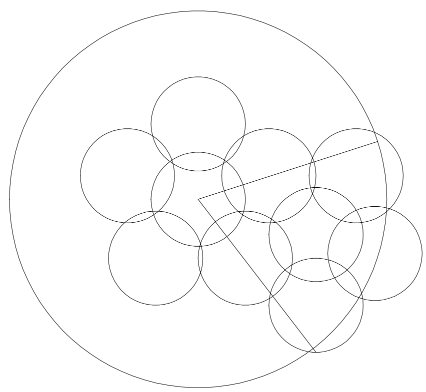

Fig. 2. Illustration of proof of Proposition 5.1. Six copies of the unit ball are used to cover the central part of $\overline{B(0,4)}$. Four more copies are needed to cover the section of angle $2\pi/5$.

Essential for the estimate of the universal upper bound K_2 was John's Theorem 3.2. Another result of John, cited in [2], is used with similar reasoning to derive that the Meyer number of centrally symmetric convex sets $\Omega \subset \mathbb{R}^2$ is bounded by 16. It is conceivable that both of these estimates on the Meyer number of two-dimensional convex compact sets are too rough. We conjecture that the maximal Meyer number is reached on a triangle.

Remark 5.2. Any triangle Ω can be transformed to an equilateral one by an affine map. Therefore it suffices to determine the Meyer number of an equilateral triangle. If Ω is such a triangle with side-length 1, then $\Omega - \Omega$ is a regular hexagon of radius 1. Figure 3 shows that thirteen open copies of the triangle Ω are sufficient to cover the closed hexagon $\Omega - \Omega$, i.e. $f(\Omega) \leq 13$.

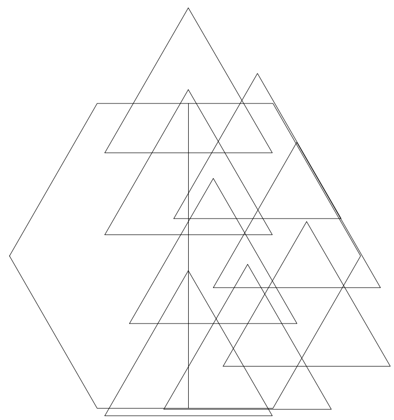

Fig. 3. Let Ω be a triangle. Then $f(\Omega) \leq 13$.

According to our knowledge, among all two–dimensional convex sets, the triangle has the largest Meyer number. On the other hand it is likely that $f(\Omega)$ is smallest for Ω being an ellipse.

Remark 5.3. For every closed ellipse E in $\mathbb{R}^2$ there exists an affine mapping such that $A(E) = \overline{B(0,1)}$. Using invariance of f under affine transformations of Ω we have $f(E) = f(A(E)) = f(\overline{B(0,1)})$. Figure 4 illustrates determining of the value of $f(\overline{B(0,1)}) = f(E) = 8$.

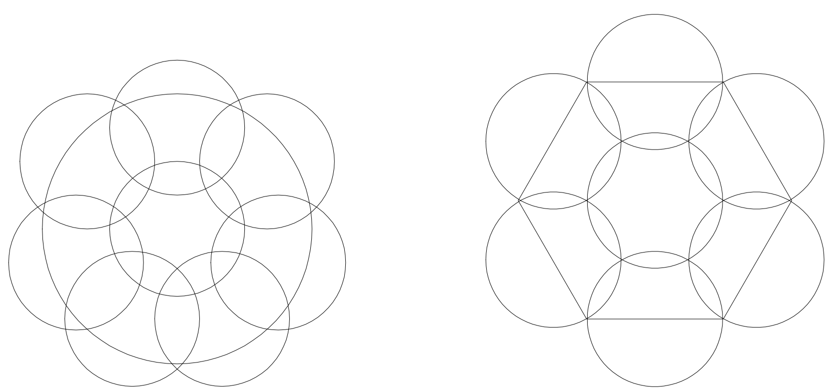

Fig. 4. The left hand part of Figure 4 shows that eight copies of a unit ball are sufficient to cover $\overline{B(0,2)}$. The right hand part of the figure illustrates that seven are not sufficient, since for covering the boundary of $\overline{B(0,2)}$ one needs six closed and not only open unit balls. This means that the Meyer number of an ellipse is equal to $f(\Omega) = 8$.

All together, we conjecture that $8 \leq f(\Omega) \leq 13$ for every convex compact set $\Omega \subset \mathbb{R}^2$.

6 Meyer number for regular polygons

It is interesting to determine the value of the function f on the simplest two–dimensional shapes, namely regular polygons. It turns out that for determining the Meyer number of regular n–gons for $n \geq 7$, one can use the following proposition taken from [2], which says that the Meyer number for every set Ω which is not 'far' from a ball is bounded by 8.

Proposition 6.1. *Let Ω be a convex compact set in $\mathbb{R}^2$ such that there exist $x, y \in \mathbb{R}^2$ and $r > 0$ satisfying $\overline{B(x, cr)} \subset \Omega^\circ \subset \overline{B(y, r)}$, where $c := 2\big(1 + 2\cos(\frac{2\pi}{7})\big)^{-1}$. Then $f(\Omega) \leq 8$.*

It remains to determine the Meyer number for the regular hexagon, pentagon and the square. We do it in a constructive way, as shown in the following remark.

Remark 6.2. Let Ω be a regular hexagon, pentagon or square. Then $f(\Omega) = 9$, as illustrated on Figure 5.

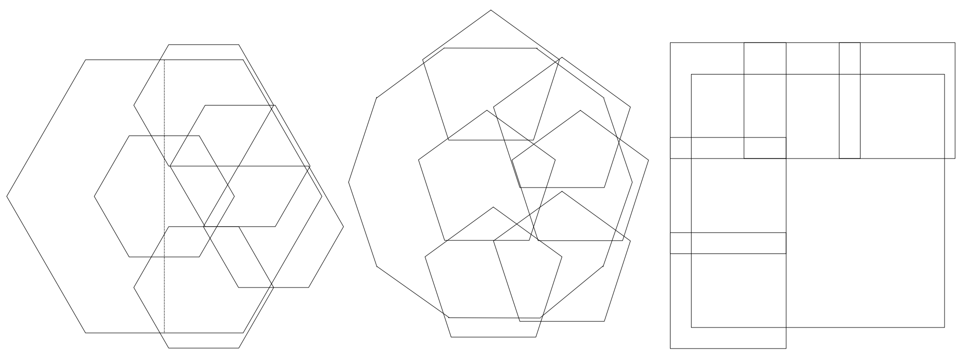

Fig. 5. Covering of the difference set $\Omega - \Omega$ by nine open copies of Ω in cases that Ω is a regular hexagon, pentagon or square.

– If Ω is a regular hexagon with the radius of escribed circle being 1, then $\Omega - \Omega$ is a regular hexagon of double size. For covering of the boundary of a closed hexagon of radius 2 one needs 8 open hexagons of radius 1. One more hexagon is used for covering the centre.

– If Ω is a regular pentagon with the radius of escribed circle being 1, then $\Omega - \Omega$ is a regular decagon of radius $1 + \frac{\sqrt{3}}{2}$. The explanation is analogous to that for hexagon.

– If Ω is a square of side–length 1, then $\Omega - \Omega$ is a square of double side-length. For covering the upper edge of the large square one needs 3 open copies of the unit square, the same number is needed for the lower edge and for the remaining part in the middle of the square.

We summarize the results about the Meyer number of regular n–gons in the following proposition.

Proposition 6.3. *Let Ω be a regular n–gon. Then $f(\Omega) \le 8$ for $n \ge 7$, $f(\Omega) = 9$ for $n = 4, 5, 6$ and $f(\Omega) \le 13$ for $n = 3$.*

7 Universal bound on the Meyer number for convex sets in $\mathbb{R}^3$

We use the same tool to find an upper bound on the Meyer number for convex $\Omega \subset \mathbb{R}^3$ as we did in the case of $\Omega \subset \mathbb{R}^2$. Theorem 3.1 claims that the universal upper bound K_3 on the Meyer number $f(\Omega)$ of convex compact sets $\Omega \subset \mathbb{R}^3$ is less or equal to the number of translated copies of the open unit ball $B(0,1)$ needed to cover the closed ball $\overline{B(0,6)}$. We estimate this number by arrangement of the centers of unit balls in a lattice so that they cover the closed ball $\overline{B(0,6)}$. We consider first the orthogonal lattice and then the orange pile arrangement. It is however conceivable that in the minimal covering the centers of unit balls do not have lattice arrangement.

Remark 7.1. For covering of $\overline{B(0,6)}$ by open translated copies of $B(0,1)$ we use first the orthogonal lattice $\left(\frac{2}{\sqrt{3}} - \varepsilon\right)\mathbb{Z}^3$ for $\varepsilon > 0$, which will be specified later. If to every lattice point $\left(\frac{2}{\sqrt{3}} - \varepsilon\right)(k, l, m)$ of norm ≤ 7 we put an open cube of side–length $\frac{2}{\sqrt{3}}$, we cover the ball $\overline{B(0,6)}$, as illustrated on Figure 6.

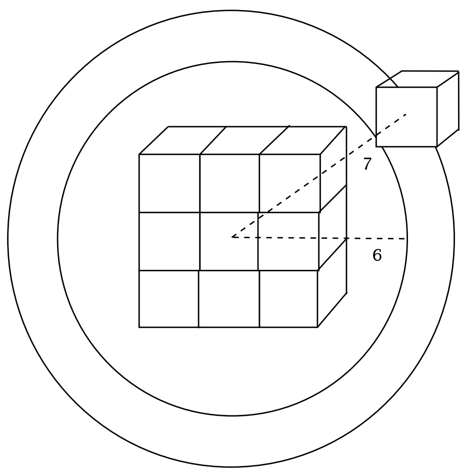

Fig. 6. Illustration of the arrangement of cubes which cover the closed ball $\overline{B(0,6)}$.

Replacing the cubes by escribed balls we obtain a covering of $\overline{B(0,6)}$ by open copies of $B(0,1)$. The number of such cubes/balls is equal to the number of all integer solutions (k, l, m) of the inequality

$$\left(\frac{2}{\sqrt{3}} - \varepsilon\right)^2 k^2 + \left(\frac{2}{\sqrt{3}} - \varepsilon\right)^2 l^2 + \left(\frac{2}{\sqrt{3}} - \varepsilon\right)^2 m^2 \le 49\,,$$

which has the same number of integer solutions as

$$k^2 + l^2 + m^2 \le \left[\left(\tfrac{2}{\sqrt{3}} - \varepsilon \right)^{-2} 49 \right] = 36$$

for sufficiently small ε. The number of such solutions is 925. Thus $f(\Omega) \le 925$ for convex Ω.

Remark 7.2. In analogy with the well known packing problem in combinatorics, where one looks for the densest packing of 3–dimensional space by non-overlapping balls, it is likely that the role of the most efficient lattice for covering will also be played by the orange pile arrangement, see Figure 7, i.e. the lattice $\mathbb{Z}x_1 + \mathbb{Z}x_2 + \mathbb{Z}x_3$, where x_1, x_2, x_3 are vectors of equal length, pairwise of angle $60°$.

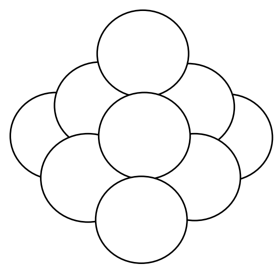

Fig. 7. Illustration of the orange pile arrangement.

For our purpose let x_1, x_2, x_3 be vectors of length $\frac{2\sqrt{2}}{\sqrt{3}} - \varepsilon$, where $\varepsilon > 0$ will be specified later. Now, we situate unit balls to all the points $kx_1 + lx_2 + mx_3$, $k, l, m \in \mathbb{Z}$, having the norm ≤ 7. As the regular tetrahedra with side–length $\frac{2\sqrt{2}}{\sqrt{3}}$ has the mass center in distance 1 of the vertices, such unit balls cover the entire closed ball $\overline{B(0,6)}$. The number of unit balls is equal to the number of integer solutions of the inequality

$$\|kx_1 + lx_2 + mx_3\| \le 7\,.$$

Taking the second power of both sides of the inequality one obtains

$$\left(\tfrac{2\sqrt{2}}{\sqrt{3}} - \varepsilon \right)^2 \left(k^2 + l^2 + m^2 + kl + lm + km \right) \le 49\,,$$

which has the same number of integer solutions as

$$k^2 + l^2 + m^2 + kl + lm + km \le \left[\left(\tfrac{2\sqrt{2}}{\sqrt{3}} - \varepsilon \right)^{-2} 49 \right] = 18$$

for sufficiently small ε. Surprisingly, the number of such solutions is again 925, thus the orange pile arrangement is in this case not more efficient than the orthogonal lattice.

Proposition 7.3. *Let Ω be a convex compact set in $\mathbb{R}^3$ with non-empty interior. Then $f(\Omega) \le 925$.*

8 Conclusion

In this paper we study the Meyer property of cut-and-project sets. Their structural complexity is dependent on the cardinality of the finite set F satisfying $\Sigma(\Omega) - \Sigma(\Omega) \subset \Sigma(\Omega) + F$. We have transformed this problem to the covering problem, i.e. to investigation of the Meyer number $f(\Omega)$ of convex compact sets $\Omega \subset \mathbb{R}^d$ defined as the minimal number of open copies Ω° needed to cover the difference set $\Omega - \Omega$. The main result is that for every dimension d there is an upper bound K_d such that $f(\Omega) \leq K_d$ for any convex compact set $\Omega \subset \mathbb{R}^d$. For estimates of K_d one needs to find the minimal covering of the closed ball $\overline{B(0,2d)} \subset \mathbb{R}^d$ by open unit balls. This may be a difficult problem in general.

We have focused on dimension $d = 2$ and shown that $f(\Omega) \leq K_2 \leq 26$ for any convex compact set $\Omega \subset \mathbb{R}^2$. It is however apparent that this bound is not reached. In order to find better estimates, we have determined the Meyer number for some special types of convex sets in $\mathbb{R}^2$. These results lead us to conjecture that $8 \leq f(\Omega) \leq 13$ for any convex compact $\Omega \subset \mathbb{R}^2$.

It is difficult to find the Meyer number even for special types of convex compact $\Omega \subset \mathbb{R}^3$. We have shown that $f(\Omega) \leq K_3 \leq 925$ for any convex compact set $\Omega \subset \mathbb{R}^3$. To obtain this estimate on the universal upper bound we used again Theorem 3.1. Situating the centers of open unit balls for covering the closed ball $\overline{B(0,6)}$ in the vertices of the orthogonal lattice, and of the orange pile lattice provides the same values. It remains an open problem whether the estimate of the universal upper bound on the Meyer number of three-dimensional convex compact sets can be refined by arrangement of ball–centers to points of another lattice.

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