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Discrete Tomography of Mathematical Quasicrystals: A Primer

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Abstract

This text is a report on work in progress. We introduce the class of cyclotomic model sets (mathematical quasicrystals) $\varLambda \subset \mathbb{Z}[\xi_n]$, where $\mathbb{Z}[\xi_n]$ is the ring of integers in the nth cyclotomic field $\mathbb{Q}(\xi_n)$, and discuss the corresponding decomposition, consistency and reconstruction problems of the discrete tomography of these sets. Our solution of the so-called decomposition problem also applies to the case of the square lattice $\mathbb{Z}^2 = \mathbb{Z}[\xi_4]$, which corresponds to the classical setting of discrete tomography.

Keywords: Consistency problem, cyclotomic model set, decomposition problem, discrete tomography, reconstruction problem.

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1 Introduction

Discrete tomography is mainly concerned with the reconstruction of a finite patch of (atomic) positions from projection data, called *X-rays*, along certain rays of parallel lines (or, more generally, from other systems of intersecting sets). In the simplest situation, the positions to be determined form a subset of the square lattice (or, more generally, of $\mathbb{Z}^d$, $d \geq 2$) and this can be considered to be the main and best understood example. In fact, most of the problems in discrete tomography have been studied on the square lattice $\mathbb{Z}^2$ (see [10]), which will be referred to as the classical case. In the longer run, one has to take into account more general classes of sets, or at least significant deviations from the lattice structure. As an intermediate step between periodic and random (or amorphous) sets, we want to investigate the discrete tomography of systems of *aperiodic order*, more precisely, of so-called *mathematical quasicrystals* (or *model sets*), which are commonly accepted to be a good mathematical model for quasicrystalline structures that appear in nature [17].

Here, we restrict ourselves to a well-known class of planar model sets, namely, using the Minkowski representation of algebraic number fields, we introduce for $n \notin \{1,2,3,4,6\}$ the corresponding class of *cyclotomic model sets* $\varLambda \subset \mathbb{Z}[\xi_n]$, where ξ_n is a primitive nth root of unity (e.g., $\xi_n = e^{\frac{2\pi i}{n}}$). The $\mathbb{Z}$-module $\mathbb{Z}[\xi_n]$ is the ring of integers in the nth cyclotomic field $\mathbb{Q}(\xi_n)$, and with the above restrictions, when viewed as a subset of the plane, is dense. Well-known examples are the planar model sets with N-fold cyclic symmetry associated with the the Ammann-Beenker tiling ($n = N = 8$), the Tübingen triangle tiling ($2n = N = 10$) and the shield tiling ($n = N = 12$). Note that $5, 8, 10$ and 12 are standard cyclic symmetries of genuine planar quasicrystals [17].

We consider the consistency and the reconstruction problem of the discrete tomography of cyclotomic model sets given X-rays in $m \geq 2$ directions and indicate that they are algorithmically solvable in polynomial time if $m = 2$. This extends well-known results from the classical case to the new setting. There are other important results concerning the classical case that can possibly be extended, e.g., the uniqueness results of Gardner and Gritzmann, compare [10, Ch. 4].

Let F be a finite subset of $t + \mathbb{Z}[\xi_n]$, where $n \geq 3$ and $t \in \mathbb{R}^2$. Furthermore, let $o \in \mathbb{Z}[\xi_n] \setminus \{0\}$ be a *module direction* (other directions are not considered for practical reasons) and let $\mathcal{L}_o$ be the set of lines in direction o in the Euclidean plane $\mathbb{R}^2$. Then, the *(discrete) X-ray of F in direction*[3] o is the function $X_o(F) : \mathcal{L}_o \longrightarrow \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, defined by

$$X_o(F)(\ell) := \left|F \cap \ell\right| = \sum_{x \in \ell} \mathbb{1}_F(x),$$

where $\mathbb{1}_F$ denotes the characteristic function of $F \subset \mathbb{R}^2$. Obviously, $X_o(F)$ has finite support $\mathrm{supp}(X_o(F))$ (the set of lines in direction o that pass through at least one point of F) and, moreover, the cardinality of F is implicit in the X-ray since we have

$$\sum_{\ell \in \mathrm{supp}(X_o(F))} X_o(F)(\ell) = \left|F\right|.$$

For the so-called *decomposition problem*, it suffices to consider the underlying $\mathbb{Z}$-modules $\mathbb{Z}[\xi_n]$ of cyclotomic model sets themselves, and, by allowing $n \in \{3, 4, 6\}$, the crystallographic cases, namely, the triangular lattice and the square lattice, are included. For a module direction o, we denote by $\mathcal{L}_o^{\mathbb{Z}[\xi_n]} \subset \mathcal{L}_o$ the set of *module lines* in direction o in the Euclidean plane $\mathbb{R}^2$, i.e., the set of lines in the Euclidean plane that are parallel to o and pass through at least one point of $\mathbb{Z}[\xi_n]$. Let $o_1, \dots, o_m \in \mathbb{Z}[\xi_n]$ be $m \geq 2$ pairwise non-parallel module directions and let $p_{o_1}, \dots, p_{o_m}$ be functions $p_{o_i} : \mathcal{L}_{o_i} \longrightarrow \mathbb{N}_0$, $i \in \{1, \dots, m\}$, whose supports are finite and satisfy

$$\mathrm{supp}(p_{o_i}) \subset \mathcal{L}_{o_i}^{\mathbb{Z}[\xi_n]},$$

$i \in \{1, \dots, m\}$. Then, the associated *grid* $\mathcal{G}_{\{p_{o_i} | i \in \{1,\dots,m\}\}}$ is defined by

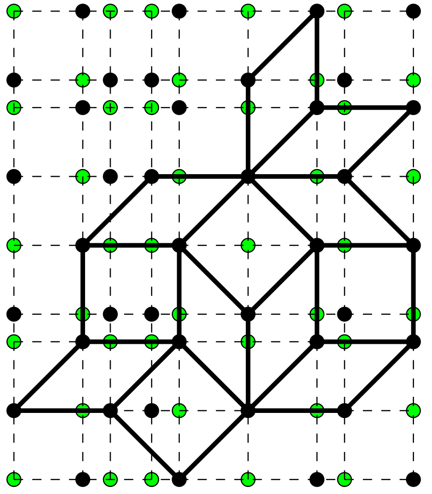
$$\mathcal{G}_{\{p_{o_i} | i \in \{1,\dots,m\}\}} := \bigcap_{i=1}^{m} \Big(\bigcup_{\ell \in \mathrm{supp}(p_{o_i})} \ell \Big).$$

We consider the phenomenon of multiple equivalence classes modulo $\mathbb{Z}[\xi_n]$ in the grid[4]. Clearly, this phenomenon affects both the consistency and the reconstruction problem, and it can also occur in the crystallographic cases $n = 3$ and $n = 4$. To see this, consider the simple situation shown in Figure 1 on the right. There, *no* translate of the marked finite subset of the square lattice is contained in any of the other equivalence classes (even when rotations or reflections of this set were allowed additionally). Alternatively, note the fact

[3] Other authors use the names projection data, marginal or line sum for this concept.

[4] Here, the equivalence relation on the grid is given by: $g \sim g' :\Longleftrightarrow g - g' \in \mathbb{Z}[\xi_n]$.

that *exactly* one of the equivalence classes (marked green) has 14 elements, whereas the remaining ones only have 13 elements; it follows that this equivalence class (which generates the same grid) would be the unique solution of the associated reconstruction problem.



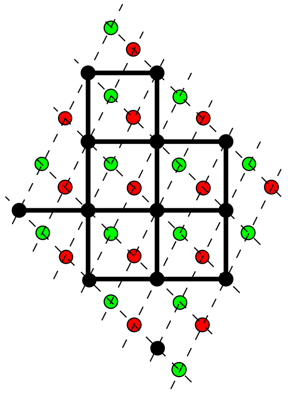


Fig. 1. Grids arising from two module directions: on the left, a finite subset (marked by the connecting lines) of the cyclotomic model set associated with the Ammann-Beenker tiling (compare Figure 2) whose grid shows 2 equivalence classes modulo $\mathbb{Z}[\xi_8]$ is shown. On the right, there is a finite subset (again marked by the connecting lines) of the square lattice with a grid containing 3 equivalence classes modulo the Gaussian integers $\mathbb{Z}[\xi_4] = \mathbb{Z}[i] = \mathbb{Z}^2$.

Hence, the problem of decomposing the grid into its equivalence classes modulo $\mathbb{Z}[\xi_n]$ is the first problem to be solved when dealing with the consistency or the reconstruction problem, also in the classical case. Using standard results from algebra, one can show that it is solvable in polynomial time. In fact, whenever the directions are fixed, it turns out that there are only *finitely* many equivalence classes. Clearly, the result extends to the case of cyclotomic model sets, which is our main interest here.

In order to describe the consistency and the reconstruction problem for the new setting, given X-rays in two module directions, let o_1, o_2 be two module directions, i.e., $o_1, o_2 \in \mathbb{Z}[\xi_n]$, with $\{o_1, o_2\}$ linearly independent over $\mathbb{R}$. Then, for the reconstruction problem, we are given two functions $p_{o_1} : \mathcal{L}_{o_1} \longrightarrow \mathbb{N}_0$

and $p_{o_2} : \mathcal{L}_{o_2} \longrightarrow \mathbb{N}_0$ whose supports are finite and satisfy

$$\mathrm{supp}(p_{o_i}) \subset \mathcal{L}_{o_i}^{\mathbb{Z}[\xi_n]},$$

$i \in \{1,2\}$. Then, the task is to construct a finite subset F which is contained in a translate of the form $t + \Lambda$, where $t \in \mathbb{R}^2$ and $\Lambda \subset \mathbb{Z}[\xi_n]$ belongs to the corresponding family of cyclotomic model sets which have, up to translation, the same *window* (see below for details), and satisfies $X_{o_1}(F) = p_{o_1}$ and $X_{o_2}(F) = p_{o_2}$ under the assumption that at least one such F exists; for the consistency problem, one merely has to answer the corresponding existency question.

The main motivation for our interest in the discrete tomography of model sets comes from the physical existence of quasicrystals that can be described as model sets and the demand of materials science to reconstruct three-dimensional (quasi)crystals from their images under high resolution transmission electron microscopy (HRTEM) in a finite and small number of module directions. At present, the measurement of the number of atoms lying on a line in a module direction can only be achieved for some crystals, see [11,16]. However, it is reasonable to expect that future developments will improve this situation.

2 Setting

For all $n \in \mathbb{N}$, and ξ_n a fixed primitive nth root of unity (e.g., $\xi_n = e^{\frac{2\pi i}{n}}$), let $\mathbb{Q}(\xi_n)$ be the corresponding cyclotomic field. Throughout this text, we will use the notation

$$\mathbb{K}_n := \mathbb{Q}(\xi_n),\ \mathcal{O}_n := \mathbb{Z}[\xi_n],$$

and ϕ will always denote Euler's totient function, i.e.,

$$\phi(n) = \left|\{k \in \mathbb{N} \,|\, 1 \leq k \leq n \text{ and } \gcd(k,n) = 1\}\right|.$$

Remark 2.1 Seen as a point set of $\mathbb{R}^2$, $\mathcal{O}_n$ has $\mathrm{lcm}(n,2)$-fold cyclic symmetry, and, except for the one-dimensional case $n \in \{1,2\}$ ($\mathcal{O}_1 = \mathcal{O}_2 = \mathbb{Z}$), the crystallographic cases $n \in \{3,6\}$ (triangular lattice) and $n = 4$ (square lattice), $\mathcal{O}_n$ is dense in $\mathbb{R}^2$.

2.1 The Class of Cyclotomic Model Sets

By definition, *model sets* arise from so-called *cut and project schemes*, compare [12]. In particular, the class of *cyclotomic* model sets arises from cut and project schemes of the following form. Let $n \in \mathbb{N} \setminus \{1,2,3,4,6\}$ and consider the following diagram (cut and project scheme), where we follow the algebraic setting of Pleasants [13].

$$
\begin{array}{ccccc}
\mathbb{R}^2 & \xleftarrow{\;\pi\;} & \mathbb{R}^2 \times (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1} & \xrightarrow{\;\pi_{\text{int}}\;} & (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1} \\
\cup\ {\scriptstyle \text{dense}} & & \cup\ {\scriptstyle \text{lattice}} & & \cup\ {\scriptstyle \text{dense}} \\
\underbrace{\mathcal{O}_n}_{=:L} & \stackrel{1-1}{\longleftrightarrow} & \underbrace{\{(z = \sigma_1(z), \underbrace{(\sigma_2(z), \dots, \sigma_{\frac{\phi(n)}{2}}(z))}_{=:z^\star}) \,|\, z \in \mathcal{O}_n\}}_{=:\tilde{L}} & \stackrel{1-1}{\longleftrightarrow} & \underbrace{(\mathcal{O}_n)^{\frac{\phi(n)}{2}-1}}_{=L^\star}
\end{array}
$$

Note that the elements of the Galois group $G(\mathbb{K}_n/\mathbb{Q}) \cong (\mathbb{Z}/n\mathbb{Z})^\times$ (where $a \pmod n$ corresponds to the automorphism given by $\xi_n \longmapsto \xi_n^a$, cf. [18, Theorem 2.5]) come in pairs of complex conjugate automorphisms. The set $\{\sigma_i \,|\, i \in \{1, \dots, \frac{\phi(n)}{2}\}\}$ arises from $G(\mathbb{K}_n/\mathbb{Q})$ by choosing exactly one automorphism of each such pair (here, we choose the identity as σ_1 rather than complex conjugation). Then, $\tilde{L}$ is a Minkowski representation of the maximal order $\mathcal{O}_n$ of $\mathbb{K}_n$, see [8, Ch. 2, Sec. 3] and [18, Theorem 2.6]. By saying that $\tilde{L}$ is a (full) lattice in

$$\mathbb{R}^2 \times (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1},$$

we mean that it is a discrete subgroup of the Abelian group $\mathbb{R}^2 \times (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}$ such that the quotient group

$$\left(\mathbb{R}^2 \times (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}\right) / \,\tilde{L}$$

is compact. This is equivalent to the existence of $\phi(n)$ $\mathbb{R}$-linearly independent vectors in $\mathbb{R}^{\phi(n)}$ whose $\mathbb{Z}$-linear hull equals $\tilde{L}$, compare [8, Ch. 2, Sec. 3 and 4]. Given any subset $W \subset (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}$ with $\varnothing \neq W^\circ \subset W \subset \overline{W^\circ}$ compact (in particular, W is relatively compact) and any $t \in \mathbb{R}^2$, we obtain a planar *model set* $\varLambda_n(t, W) := t + \varLambda_n(W)$ relative to the above cut and project scheme by setting

$$\varLambda_n(W) := \{z \in \mathcal{O}_n \,|\, z^\star \in W\},$$

compare [12,13] for details and more general settings, and [7] for general background. Further, $\mathbb{R}^2$ (resp. $(\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}$) is called the *physical* (resp. *internal*) space, W is referred to as the *window* of $\varLambda_n(t, W)$ and

$$^\star\colon\; L \longrightarrow (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}$$

is the so-called *star* map. Then, $\varLambda_n(t, W) \subset \mathbb{R}^2$ is a *Delone* set (i.e., $\varLambda_n(t, W)$ is both uniformly discrete and relatively dense), has *finite local complexity* and is *aperiodic* (i.e., $\varLambda_n(t, W)$ has no translational symmetries), compare [12] again. Moreover, if $\varLambda_n(t, W)$ is *regular* (i.e., if the boundary ∂W has measure 0 in $(\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}$), then $\varLambda_n(t, W)$ is *pure point diffractive* (cf. [15]), and if $\varLambda_n(t, W)$ is *generic* (i.e., if $L^\star \cap \partial W = \varnothing$), then $\varLambda_n(t, W)$ is *repetitive*, see [15]. If $\varLambda_n(t, W)$ is both generic and regular, the frequency of repetition is well-defined (cf. [14]) and, moreover, $\varLambda_n(t, W)$ has $\operatorname{lcm}(n, 2)$-fold cyclic symmetry in the sense of symmetries of LI-classes, see [2] for details and compare Remark 2.1.

For any $n \in \mathbb{N} \setminus \{1, 2, 3, 4, 6\}$, set

$$\begin{aligned}&\mathcal{M}(\mathcal{O}_n) :=\\ &\{\varLambda_n(t, W) \,|\, t \in \mathbb{R}^2, W \subset (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1} \text{ with } \varnothing \neq W^\circ \subset W \subset \overline{W^\circ} \text{ compact}\}.\end{aligned}$$

Then, the class $\mathcal{CM}$ of *cyclotomic* model sets is defined as the union of all sets $\mathcal{M}(\mathcal{O}_n)$, i.e.,

$$\mathcal{CM} := \bigcup_{n \in \mathbb{N}\setminus\{1,2,3,4,6\}} \mathcal{M}(\mathcal{O}_n).$$

2.2 Examples

All examples below are of the form $\varLambda_n(0, W)$ for suitable $n \in \mathbb{N}\setminus\{1, 2, 3, 4, 6\}$.

(a) The planar generic regular model set with 8-fold cyclic symmetry associated with the well-known Ammann-Beenker tiling [1,4,9] can be described in algebraic terms as

$$\varLambda_{\mathrm{AB}} := \{z \in \mathcal{O}_8 \,|\, z^\star \in O\},$$

where the star map * is the Galois automorphism in $G(\mathbb{K}_8/\mathbb{Q})$, defined by $\xi_8 \longmapsto \xi_8^3$, and the window O is the regular octagon centred at the origin and of unit edge length with orientation as in Figure 2. This construction also gives a tiling with squares and rhombi, both having edge length 1, see Figure 2.

(b) The planar regular model set with 10-fold cyclic symmetry associated with the Tübingen triangle tiling [5,6] can be described in algebraic terms

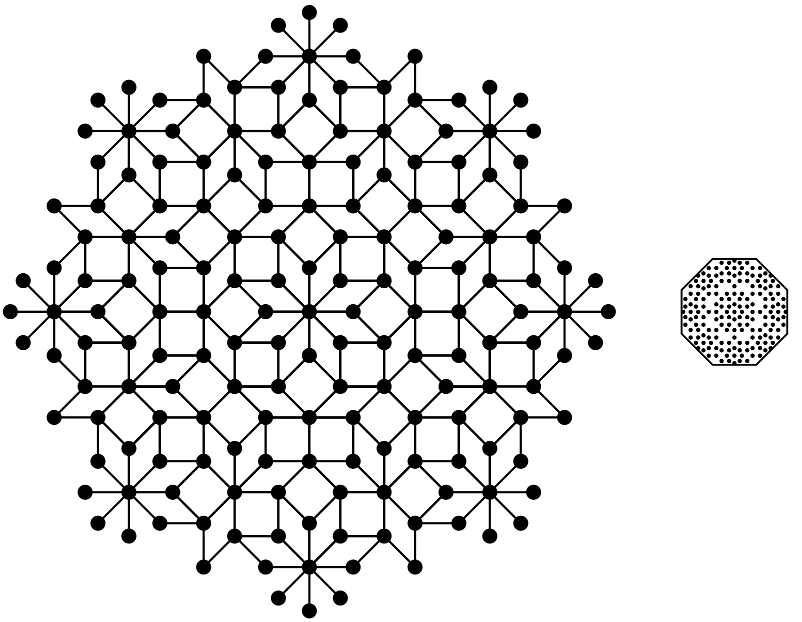


Fig. 2. A central patch of the eightfold symmetric Ammann-Beenker tiling with vertex set $\varLambda_{\mathrm{AB}}$ (left) and the *-image of $\varLambda_{\mathrm{AB}}$ inside the octagonal window in the so-called internal space (right), with relative scale as described in the text.

as

$$\varLambda_{\mathrm{TTT}} := \{z \in \mathcal{O}_5 \,|\, z^\star \in W\},$$

where the star map * is the Galois automorphism in $G(\mathbb{K}_5/\mathbb{Q})$, defined by $\xi_5 \longmapsto \xi_5^2$, and the window W is the regular decagon centred at the origin, with vertices in the directions that arise from the 10th roots of unity by a rotation through $\frac{\pi}{10}$, and of edge length $\frac{\tau}{\sqrt{\tau+2}}$, where τ is the golden ratio, i.e., $\tau = \frac{\sqrt{5}+1}{2}$. This construction gives a triangle tiling with long (short) edges of lengths 1 ($\frac{1}{\tau}$), see Figure 3 for a repetitive example, obtained by a tiny shift of the window into a generic position.

(c) The planar regular model set with 12-fold cyclic symmetry associated with the shield tiling [9] can be described in algebraic terms as

$$\varLambda_{\mathrm{S}} := \{z \in \mathcal{O}_{12} \,|\, z^\star \in W\},$$

where the star map * is the Galois automorphism in $G(\mathbb{K}_{12}/\mathbb{Q})$, defined by $\xi_{12} \longmapsto \xi_{12}^5$, and the window W is the regular dodecagon centred at the origin, with vertices in the directions that arise from the 12th roots of

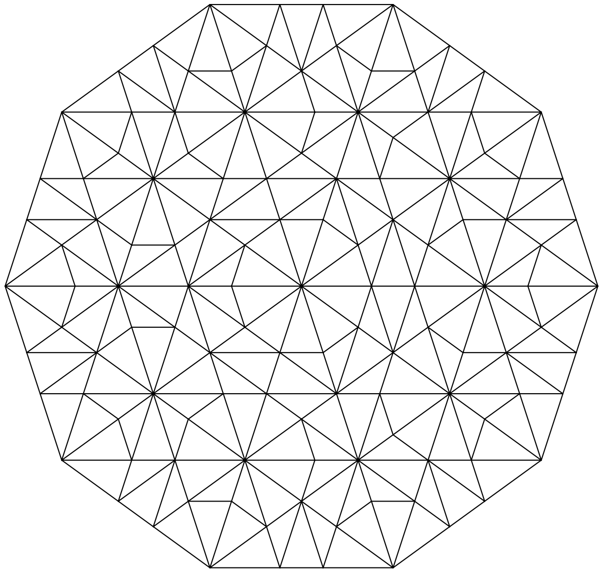


Fig. 3. A central patch of the tenfold symmetric Tübingen triangle tiling.

unity by a rotation through $\frac{\pi}{12}$, and of edge length 1. This construction gives a tiling with triangles, squares and so-called shields, all having edge length $\frac{\sqrt{3}-1}{\sqrt{2}}$, see Figure 4 for a repetitive example, once again obtained by a tiny shift of W into a generic position.

3 Results

3.1 The Decomposition, Consistency and Reconstruction Problems

Using standard results from algebra, one can show the following result which immediately implies that both the decomposition problem of the discrete tomography of cyclotomic model sets and the corresponding problem in the classical case are tractable:

Theorem 3.1 *(cf. [3]) Let $n \geq 3$ and $o_1, \dots, o_m \in \mathcal{O}_n$ be $m \geq 2$ pairwise non-parallel module directions. Further, let $p_{o_i} : \mathcal{L}_{o_i} \longrightarrow \mathbb{N}_0$, $i \in \{1, \dots, m\}$, be functions whose supports are finite and satisfy $\mathrm{supp}(p_{o_i}) \subset \mathcal{L}_{o_i}^{\mathcal{O}_n}$, $i \in \{1, \dots, m\}$.*

Then, the problem of decomposing the associated grid $\mathcal{G}_{\{p_{o_i} | i \in \{1,\dots,m\}\}}$ (cf. Section 1) into its equivalence classes modulo $\mathcal{O}_n$ can be solved in polynomial time. □

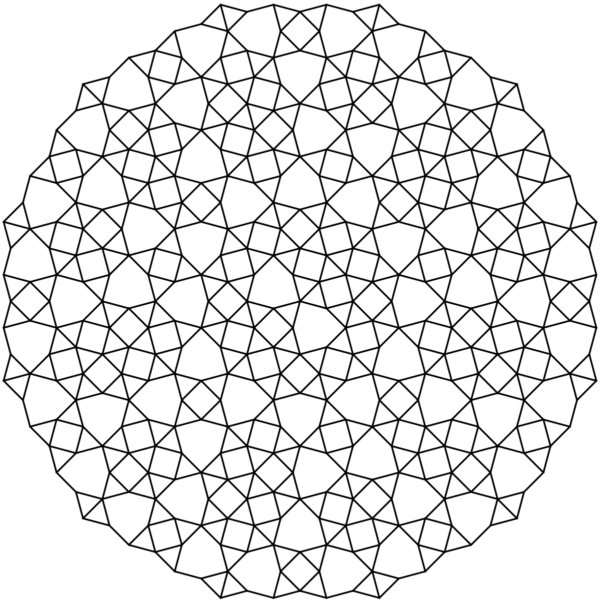


Fig. 4. A central patch of the twelvefold symmetric shield tiling.

Remark 3.2 In fact, in the situation of Theorem 3.1, it turns out that, whenever the module directions are fixed, there are only *finitely* many equivalence classes. Depending on the functions p_{o_i}, not all of them may be present.

Next, we turn to the consistency and reconstruction problems, given X-rays in *two* module directions. More precisely, for the reconstruction problem, we are given an $n \in \mathbb{N} \setminus \{1,2,3,4,6\}$, two non-parallel module directions $o_1, o_2 \in \mathcal{O}_n$, two functions $p_{o_1} : \mathcal{L}_{o_1} \longrightarrow \mathbb{N}_0$, $p_{o_2} : \mathcal{L}_{o_2} \longrightarrow \mathbb{N}_0$ whose supports are finite and satisfy $\mathrm{supp}(p_{o_i}) \subset \mathcal{L}_{o_i}^{\mathcal{O}_n}$, $i \in \{1,2\}$. Moreover, we are given a window $W \subset (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}$ (i.e., a set with $\varnothing \neq W^\circ \subset W \subset \overline{W^\circ}$ compact). Then, the task is to construct a finite set F which is contained in a cyclotomic model set $\varLambda_n(t, \tau + W) \in \mathcal{M}(\mathcal{O}_n)$, where $t \in \mathbb{R}^2$ and $\tau \in (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}$, and satisfies $X_{o_1}(F) = p_{o_1}$ and $X_{o_2}(F) = p_{o_2}$ under the assumption that at least one such F exists; for the consistency problem, one has to answer the corresponding existence question.

Here, we concentrate on the key problem, presently ignoring the missing steps towards a solution of the above problems.

By Theorem 3.1, we can assume that the equivalence classes of the grid $\mathcal{G}_{\{p_{o_1}, p_{o_2}\}}$ modulo $\mathcal{O}_n$ are given, say $\mathcal{G}_{\{p_{o_1}, p_{o_2}\}} = \dot{\cup}_{i=1}^{c} G_i$ (cf. Remark 3.2), where

$G_i - t_i \subset \mathcal{O}_n$ for suitable $t_i \in \mathbb{R}^2$. Let us now consider a fixed equivalence class G_i. Due to the definition of (cyclotomic) model sets, not every subset of G_i that conforms to the X-rays is admissible, more precisely: a possible reconstruction $F \subset G_i$ must satisfy:

$$\exists\, \tau \in (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1} \ : \ (F - t_i)^\star \subset \tau + W.$$

Therefore, one has to determine the set

$$\mathrm{Sep}_W((G_i - t_i)^\star) := \{(G_i - t_i)^\star \cap (\tau + W) \,|\, \tau \in (\mathbb{R}^2)^{\frac{\phi(n)}{2}-1}\},$$

which contains all those subsets of $(G_i - t_i)^\star$ that are "separable" from its complement by a translate of W.

This problem is tractable for special classes of windows:

Theorem 3.3 *(cf. [3]) Let $P \subset \mathbb{R}^d$ be a finite set. Then, one has:*

(a) If W is a ball of fixed radius in $\mathbb{R}^d$, then the determination of $\mathrm{Sep}_W(P) = \{P \cap (\tau + W) \,|\, \tau \in \mathbb{R}^d\}$ can be done with $\mathcal{O}((\mathrm{card}(P))^{d+2})$ arithmetic operations.

(b) If $W = \{x \in \mathbb{R}^d \,|\, Ax \leq b\}$ is a fulldimensional polytope in $\mathbb{R}^d$, then the determination of $\mathrm{Sep}_W(P)$ can be done with $\mathcal{O}((\mathrm{card}(P))^{d+1})$ arithmetic operations. □

In [3], we will also give a description of the set of solutions of the above reconstruction problem.

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