Description of Voronoi tiles in quasicrystals with octagonal symmetry

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Abstract. We describe families of Voronoi tiles which appear in tilings of certain standard quasicrystal-like point sets with octagonal symmetry built using the cut-and-project construction.

1. Introduction
The description of local configurations of atomic positions or atomic clusters in quasicrystal materials is crucial for the study of their physical properties. In a mathematical model, the nearest neighbours of a given point can be described using the so-called Voronoi cell. Together, Voronoi cells of all points of the model form a perfect tiling of the space. The Voronoi tiling can be defined for point sets satisfying the Delone property defined for example by the cut-and-project construction [1]. Here we consider planar cut-and-project sets with octagonal symmetry, modelling certain experimentally observed alloys which reveal such a symmetry [2]. The acceptance window of the considered models is a regular octagon of any size. Our main goal is the description of all types of Voronoi tiles in the Voronoi tiling of such a cut-and-project set. Similar analysis has been performed for quasicrystal models with decagonal symmetry in [3] and used in cluster-based models of decagonal aluminium alloys [4].

Our task cannot be solved by observation only. Some of the tiles may occur with very low frequency, which means that they may not appear in a chosen section of the space of a given size. For a complete classification of cut-and-project models according to their families of Voronoi tiles such an analysis must be done for an uncountable number of cases (arbitrary size of the acceptance window). We present here a short overview of the results of a detailed analysis and extensive computation which allowed us to solve the question exactly. Full details of both the analysis and computations will appear in an upcoming paper. Our computation discovers even the tiles which occur with frequency close to zero. Some of the methods follow the techniques presented in [5].

2. Theory
The cut-and-project construction of the octagonal model uses projection of the root lattice of type $B_4$. Here we follow the algebraic formalism of [6], based on the 8-th cyclotomic field and the Pisot-cyclotomic number $\beta = 1 + \sqrt{2}$. 
Denote by \( \mathbb{Z}[\beta] \) the extension ring \( \mathbb{Z}[\beta] = \mathbb{Z} + \beta\mathbb{Z} \) and by \( ' \) the Galois automorphism on \( \mathbb{Z}[\beta] \) defined by \( x = a + b\beta \mapsto x' = a + b\beta' \), where \( \beta' = 1 - \sqrt{2} = -1/\beta \) is the Galois conjugate of \( \beta \). Let \( \zeta = e^{2\pi i/8}, \alpha_1 = (1, 0), \alpha_2 = (\frac{R_\zeta}{\zeta}, \frac{\Re\zeta}{\zeta}), \alpha'_1 = (0, 1), \) and \( \alpha'_2 = (\frac{\Re\zeta}{\zeta}, \frac{\Im\zeta}{\zeta}) \). The cut-and-project quasicrystal is then defined using \( \mathbb{Z} \)-modules \( M = \mathbb{Z}[\beta]\alpha_1 + \mathbb{Z}[\beta]\alpha_2 \), \( M^* = \mathbb{Z}[\beta]\alpha'_1 + \mathbb{Z}[\beta]\alpha'_2 \) and the star map \( * : M \mapsto M^* \) given by \( x = x_1\alpha_1 + x_2\alpha_2 \mapsto x' = x'_1\alpha'_1 + x'_2\alpha'_2 \).

Let \( \Omega \subset \mathbb{R}^2 \) be a bounded set with non-empty interior. The cut-and-project quasicrystal with acceptance window \( \Omega \) is the set
\[
\Sigma(\Omega) = \{ x \in M \mid x^* \in \Omega \}.
\]

Here, we consider only one type of acceptance window, namely regular octagons of any size. The size is determined by the diameters of their circumcircle.

Let \( \Sigma(\Omega) \) be a quasicrystal and let \( x \in \Sigma(\Omega) \). The Voronoi tile of \( x \) in \( \Sigma(\Omega) \) is the set of all points in the plane closer to \( x \) than to any other element of \( \Sigma(\Omega) \). Formally,
\[
V(x) = \{ y \in \mathbb{R}^n \mid \forall z \in \Sigma(\Omega), z \neq x : \|y - x\| \leq \|y - z\| \}.
\]

There are several important properties of \( \Sigma(\Omega) \), two of which are very useful for our analysis of Voronoi tiles:

(i) \( \Sigma(\Omega) \) is a Delone set, in particular it is a relatively dense set, i.e., there exists a constant \( 0 < R < \infty \) such that every ball of radius \( R \) contains at least one point of \( \Sigma(\Omega) \). The minimal \( R \) with this property is called the covering radius of \( \Sigma(\Omega) \), denoted \( R_C \). It can be shown [7] that the Voronoi cell \( V(x) \) is determined only by points of \( \Sigma(\Omega) \) within a distance of \( 2R_C \) from \( x \).

(ii) \( \Sigma(\Omega) \) satisfies the scaling property, namely that \( \beta \Sigma(\Omega) = \Sigma(\beta'\Omega) \). Thus in all our considerations we can restrict ourselves to windows (octagons) of diameters in \( (1, \beta] \).

3. Results

In Figure 1 we display the shapes of all Voronoi tiles appearing in cut-and-project quasicrystal (based on \( \beta = 1 + \sqrt{2} \)) with an acceptance window in the shape of a regular octagon. Each tile \( V(x) \) is drawn together with the points of \( \Sigma(\Omega) \) within the distance of \( 2R_C \) from \( x \), i.e., with the points determining the shape of the tile. Note that even though each tile may appear in up to 16 possible orientations (due to the action of the 16 elements of the dihedral group \( D_{16} \) – the symmetry group of the octagon) Figure 1 shows only one representative of each tile.

Thanks to the scaling property, we can restrict ourselves to octagons of diameters (strictly speaking diameters of their circumcircles) in \( (1, \beta] \). This interval can be covered by subintervals based on sets of tiles in corresponding quasicrystals, i.e., if two quasicrystals have diameters from the same subinterval then they have the same set of tiles. There are twelve such intervals \( I_1, \ldots, I_{12} \). For each \( i = 1, \ldots, 12 \) we have \( I_i = (E_{2i-1}, E_{2i+1}) \), the endpoints are listed in Table 1.

Our results can be found in Table 2 which lists all the Voronoi tiles appearing in a quasicrystal with given diameter. In odd columns there are sets of tiles in quasicrystals with diameters \( E_i \). Note that is it not necessary write down the tiles in quasicrystal with diameter \( E_{25} \) since its tiles are only rescaled versions of tiles appearing in \( E_1 \). In even columns there are sets of tiles in quasicrystals with diameters in \( I_{i/2} \). The symbols \( (\bullet) \) and \( (\circ) \) mean that the given tile does appear in the given quasicrystal, however tiles marked with \( (\circ) \) appear only with zero frequency.

Acknowledgments

This work was supported by the project CZ.02.1.01/0.0/0.0/16_019/0000778 from European Regional Development Fund.
Figure 1. Voronoi tiles in octagonal quasicrystals, numbers correspond to rows of Table 2.

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Table 1. Endpoints of intervals distinguishing quasicrystals with different sets of tiles.

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| E₁ | E₃ | E₅ | E₇ | E₉ | E₁₁ | E₁₃ | E₁₅ | E₁₇ | E₁₉ | E₂₁ | E₂₃ | E₂₅ |
| 1 | 5β - 11 | \( \frac{3β - 5}{2} \) | \( \frac{β}{2} \) | 3-β | \( \frac{β+1}{2} \) | 2 | \( \frac{3β - 3}{2} \) | \( \frac{β+2}{2} \) | 3β - 5 | \( \frac{7-β}{2} \) | β |

Table 2. Assignment of Voronoi tiles to quasicrystals according to the size of their acceptance windows.