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LETTER TO THE EDITOR

Dualisation of Voronoi domains and Klotz construction: a general method for the generation of proper space fillings

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Abstract. We present a general method for the generation of proper space fillings of Euclidean spaces with convex polytopes by projection from higher-dimensional spaces. As a special case, quasiperiodic tilings are obtained by the projection of periodic structures. The concept is general enough for the treatment of defects in quasiperiodic tilings by placing defects in high-dimensional translation lattices.

Quasiperiodic geometric structures have attracted a lot of interest since the discovery of quasicrystals in Nature [1]. The simplest examples are quasiperiodic point sets in 3-space which may serve as positions of atoms in order to model quasicrystals theoretically. Structures of this kind are usually generated by so-called cut-and-project methods projecting points of a high-dimensional point lattice into a subspace which has irrational slopes with respect to the lattice. However, these schemes suffer from a certain degree of arbitrariness. For example, the selection of the lattice points which are projected ('cut window') is not determined without additional assumptions. Furthermore, one may ask whether it is possible to take over more geometric information from the high-dimensional lattice to the quasilattice. Therefore, it is necessary to analyse the geometric structures in more detail.

The basic concept in the description of periodic structures is the unit cell. The extension of this concept to quasiperiodic structures leads to the idea of quasiperiodic tilings. Many schemes have been proposed for obtaining such tilings from a point lattice in higher dimensions. Among these are the grid and dualisation methods. But up to now, there are two disadvantages in these constructions. First of all, they essentially deal only with hypercubic lattices. Secondly, they tend to break down if one places defects into the high-dimensional lattice.

Since there is no justification for a limitation to hypercubic lattices and, on the other hand, a theory of defects in quasicrystals would be more satisfactory in the same framework as the construction of the ideal quasicrystal, one would like to have a construction method which is as general as possible.

The aim of this letter is the introduction of a scheme for generating proper space fillings which does not suffer from the disadvantages mentioned. We limit ourselves here to the presentation of the results, leaving detailed proofs to a forthcoming publication.

We first set up some basic notation and definitions which will be used throughout.

The whole construction takes place in a vector space of finite dimension n, denoted by V, which is provided with a positive definite scalar product $\cdot$ together with the

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induced norm $\|\cdot\|$ and topology. For $S_1, S_2 \subseteq V$, we write $S_1 \perp S_2$ if $x_i, y_i \in S_i$ $(i=1,2)$ implies $(x_1-y_1)\cdot(x_2-y_2)=0$.

If S is a subset of V, the convex hull of S, conv(S), is the smallest convex subset of V which contains S.

We assume that it is at least intuitively known what convex polytopes exist in V and what their bounding polytopes are. It is immediately obvious that for every finite subset $M \neq \emptyset$ of V the set conv(M) is a convex polytope in V (in fact, one may define convex polytopes this way).

For brevity, we call a bounding polytope of a (convex) polytope P a boundary of P, or more precisely, m-boundary of P if it is of dimension m. (Note that we use 'boundary' not in the usual point-set topological sense.) We include P in the set of its boundaries.

A set $\mathcal{F}$ of m-dimensional polytopes in an m-dimensional Euclidean vector space V' is called a *proper space filling* of V', if the following two conditions hold.

Condition F1: $V' = \bigcup \mathcal{F}$.

Condition F2: Different elements of $\mathcal{F}$ do not intersect at interior points.

If the elements of $\mathcal{F}$ can be generated as images of finitely many polytopes from $\mathcal{F}$ under convenient translations, $\mathcal{F}$ is called a *tiling* of V'.

Of special importance is the concept of *Voronoi domains*. If Γ is an arbitrary point set in V and $q \in \Gamma$, the Voronoi domain of q with respect to Γ is the set

$$V_\Gamma(q) := \{x \in V \mid q' \in \Gamma \Rightarrow \|x-q'\| \geq \|x-q\|\}. \tag{1}$$

It is clear from the definition that $V_\Gamma(q)$ is a closed convex subset of V. In the following, we assume that Γ fulfils the following two conditions.

Condition A1: Γ has no points of accumulation in V.

Condition A2: conv$(\Gamma) = V$.

Then, it is easy to show that all $V_\Gamma(q)$ are convex polytopes in V of dimension n.

We will use the notation

$$\begin{aligned} \mathcal{V}_\Gamma &:= \{P \subseteq V \mid P \text{ is a boundary of some } V_\Gamma(q), q \in \Gamma\} \\ \mathcal{V}_\Gamma^m &:= \{P \in \mathcal{V}_\Gamma \mid \dim P = m\} \qquad 0 \leq m \leq n. \end{aligned} \tag{2}$$

For example, $\mathcal{V}_\Gamma^n$ is the set of all Voronoi domains $V_\Gamma(q)$ $(q \in \Gamma)$, while $\mathcal{V}_\Gamma^0$ is the set of all sets of the form $\{x\}$, x being a vertex of some $V_\Gamma(q)$ $(q \in \Gamma)$.

The set $\mathcal{V}_\Gamma$ is a proper space filling of V and has properties very similar to those of the well known simplicial complexes used in algebraic topology [page 7 of 2], as set out below.

Property C1: $P_1 \in \mathcal{V}_\Gamma$ $\quad$ P_2 boundary of $P_1 \Rightarrow P_2 \in \mathcal{V}_\Gamma$

Property C2: $P_1, P_2 \in \mathcal{V}_\Gamma$ $\quad$ $P_1 \cap P_2 \neq \emptyset \Rightarrow P_1 \cap P_2$ boundary of both P_1, P_2.

In other words, all boundaries of an element of $\mathcal{V}_\Gamma$ are contained in $\mathcal{V}_\Gamma$ and the polytopes of $\mathcal{V}_\Gamma$ are in 'face-to-face' relation. For that reason we call $\mathcal{V}_\Gamma$ the *Voronoi complex* associated with Γ.

Let $\Gamma \subseteq V$ fulfil conditions A1 and A2. For $P \in \mathcal{V}_\Gamma$, the set

$$M_\Gamma^*(P) := \{q \in \Gamma \mid P \subseteq V_\Gamma(q)\} \tag{3}$$

is finite. We define the *dual* P^* of P to be the convex polytope

$$P^* := \mathrm{conv}(M^*(P)). \tag{4}$$

It turns out that $\dim P^* = n - \dim P$ and $P^* \perp P$. Furthermore, if Q is a boundary of P^* $(P \in \mathcal{V}_\Gamma)$, then there exists a $P' \in \mathcal{V}_\Gamma$ such that $Q = (P')^*$. We denote

$$\mathcal{V}_\Gamma^* := \{P^* \mid P \in \mathcal{V}_\Gamma\} \qquad \mathcal{V}_\Gamma^{*m} := \{P^* \in \mathcal{V}_\Gamma^* \mid \dim P^* = m\}. \tag{5}$$

One can show that properties C1 and C2 hold for $\mathcal{V}_\Gamma^*$, so we call $\mathcal{V}_\Gamma^*$ the *dual complex* associated with Γ.

The duality relation $P \leftrightarrow P^*$ induces a one-to-one correspondence between the two complexes $\mathcal{V}_\Gamma$ and $\mathcal{V}_\Gamma^*$ which respects the bounding property as follows:

$$P_1 \subseteq P_2 \Leftrightarrow P_1^* \supseteq P_2^* \qquad P_1, P_2 \in \mathcal{V}_\Gamma \tag{6}$$

i.e., if P_1 is a boundary of P_2, then P_2^* is a boundary of P_1^*, and vice versa.

Let Γ fulfil conditions A1 and A2. We fix a linear subspace $V_\parallel$ (the 'physical' space) of V, $m := \dim V_\parallel$. There is a unique decomposition $V = V_\parallel \oplus V_\perp$, $V_\parallel \perp V_\perp$. Furthermore, $V_\parallel$ determines the orthogonal projections

$$\pi_\parallel : V \to V_\parallel \qquad \pi_\perp : V \to V_\perp .$$

For $P \in \mathcal{V}_\Gamma^m$, the *Klotz* $K(P)$ is defined by

$$K(P) := \pi_\parallel^{-1}(\pi_\parallel(P)) \cap \pi_\perp^{-1}(\pi_\perp(P^*)) = \pi_\parallel(P) + \pi_\perp(P^*). \tag{7}$$

$K(P)$ is a convex polytope in V. We call $K(P)$ non-degenerate, if $\dim(K(P)) = n$. This is the case if and only if $\dim(\pi_\parallel(P)) = m$ or, equivalently, $\dim(\pi_\perp(P^*)) = n - m$.

Let $\mathcal{K}(\Gamma, V_\parallel)$ be the set of all non-degenerate $K(P)$, $P \in \mathcal{V}_\Gamma^m$. We refer to $\mathcal{K}(\Gamma, V_\parallel)$ as the *Klotz construction* for Γ adapted to $V_\parallel$. It is obvious that $\mathcal{K}(\Gamma, V_\parallel)$ is dependent on the scalar product in V, so one can generate several Koltz constructions from one point set Γ in V by choosing different scalar products. This possibility can be advantageous, e.g., if one studies inflation rules for quasiperiodic patterns obtained by a Klotz construction.

Our main result is that $\mathcal{K}(\Gamma, V_\parallel)$ *is always a proper space filling of V if Γ fulfils the weak conditions A1 and A2.*

This yields the possibility of constructing proper space fillings in $V_\parallel$ and $V_\perp$ by some projection images $\pi_\parallel(P)$, $\pi_\perp(P^*)$, respectively $(P \in \mathcal{V}_\Gamma^m)$. To this end, choose $c_\perp \in V_\perp$ but not contained in the projection image of an l boundary $(l < n - m)$ of a $P^* \in \mathcal{V}_\Gamma^{*n-m}$ in $V_\perp$ (this holds for every $c_\perp \in V_\perp$ except for a set of measure zero with respect to some Lebesgue measure in $V_\perp$). Then the affine space $c_\perp + V_\parallel$ is properly filled by its cuts through the elements of $\mathcal{K}(\Gamma, V_\parallel)$. Shifting this into $V_\parallel$ yields the desired space filling of $V_\parallel$. As a consequence of the construction, all the polytopes that constitute this space filling are of the form $\pi_\parallel(P)$, $P \in \mathcal{V}_\Gamma^m$. The space filling of $V_\parallel$ obtained in this way is, written explicitly,

$$\mathcal{F}(\Gamma, V_\parallel, c_\perp) = \{\pi_\parallel(P) \mid P \in \mathcal{V}_\Gamma^m, K(P) \in \mathcal{K}(\Gamma, V_\parallel), c_\perp \in \pi_\perp(P^*)\}. \tag{8}$$

In an analogous fashion, for $c_\parallel \in V_\parallel$ (with a similar restriction as for $c_\perp$) one obtains a proper space filling of $V_\perp$ by projection images $\pi_\perp(P^*)$, $P \in \mathcal{V}_\Gamma^m$:

$$\mathcal{F}^*(\Gamma, V_\parallel, c_\parallel) = \{\pi_\perp(P^*) \mid P \in \mathcal{V}_\Gamma^m, K(P) \in \mathcal{K}(\Gamma, V_\parallel), c_\parallel \in \pi_\parallel(P)\}. \tag{9}$$

Let us consider the special case that Γ is a point lattice in V (i.e. the orbit of a fixed point under the translations by elements of a discrete additive subgroup $\mathcal{T}$ of V which spans V over $\mathbb{R}$). Obviously, Γ fulfils conditions A1 and A2, so Klotz constructions are possible.

In this case, as follows immediately from the very construction, every Klotz construction for Γ is invariant under translations by elements of $\mathcal{T}$, i.e. it is periodic. Therefore, one can always find finitely many $P_1, \ldots, P_k \in \mathcal{V}_\Gamma^m$ such that

$$\mathcal{K}(\Gamma, V_\parallel) = \{t + K(P_j) \mid t \in \mathcal{T}, j = 1, \ldots, k\} \tag{10}$$

(of course, as for the Klotz construction itself, the set $\{P_1, \ldots, P_k\}$ depends on $V_\parallel$ (and on the scalar product)). As a consequence, a proper space filling of $V_\parallel$ or $V_\perp$ obtained by our method will be a tiling of $V_\parallel$. For a general $V_\parallel$ in V, this tiling will not be periodic but quasiperiodic in the sense that every finite part of it will be repeated uniformly distributed over $V_\parallel$.

An example of a Klotz construction in a 2D point lattice is seen in figure 1. One observes at once that three Klötze form a fundamental domain for the 2D lattice. A cut through the construction parallel to $V_\parallel$ or $V_\perp$ yields one-dimensional tilings with three non-congruent tiles corresponding to (8) and (9), respectively.

Figure 2 shows the Klotz construction in a tetragonal lattice with one defect according to the rules presented above. Dependent on the distance of the cut plane from the defect location, there will be a local perturbation in the quasiperiodic pattern in comparison with the 'ideal' tiling. One learns from this example that local defects in the high-dimensional structure produce local defects in the projected pattern.

Let us comment on how the most familiar examples of quasiperiodic tilings fit into the framework of the Klotz construction.

The Penrose pattern in two dimensions and the icosahedral pattern in three dimensions can be obtained from hypercubic lattices in five and six dimensions, respectively. de Bruijn [3], in his analysis of the Penrose tiling, introduced a two-dimensional pentagrid and its dualisation. The grid method was generalised and

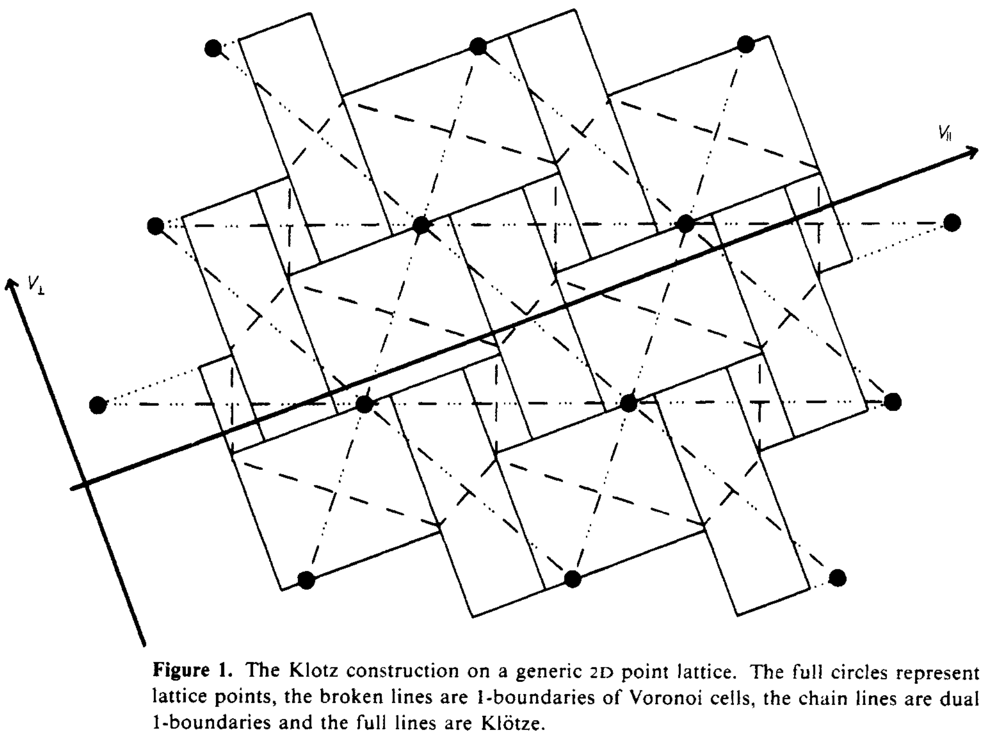

Figure 1. The Klotz construction on a generic 2D point lattice. The full circles represent lattice points, the broken lines are 1-boundaries of Voronoi cells, the chain lines are dual 1-boundaries and the full lines are Klötze.

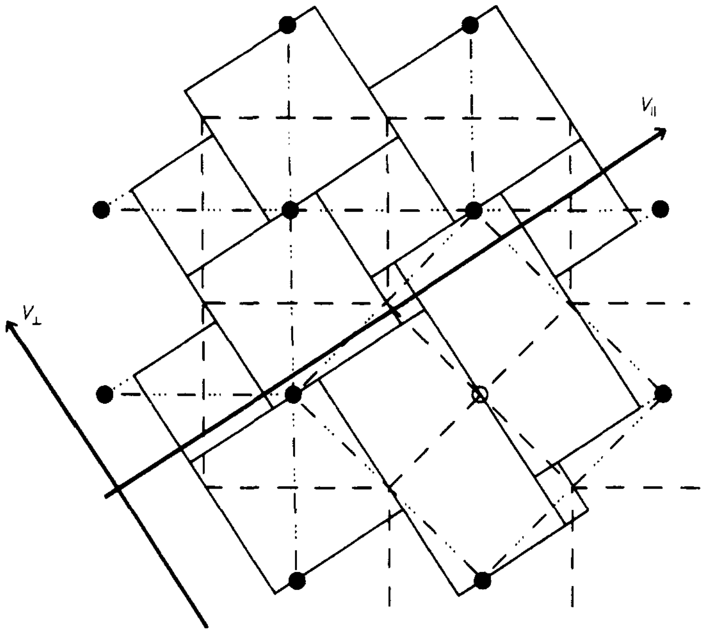

Figure 2. The Klotz construction in a tetragonal point lattice with one point removed. The full circles represent lattice points, the open circle is the removed point, the broken lines are 1-boundaries of Voronoi cells, the chain lines are dual 1-boundaries and the full lines are Klötze.

applied to the icosahedral quasilattice in three dimensions by Kramer and Neri [4]. The equivalence of the grid formalism with the strip method was shown by Gähler and Rhyner [5]. In [6] it was shown that the grid method in m-dimensional spaces arises from the duality concept for hypercubic lattices in n dimensions ($n > m$). For these lattices, the Wigner–Seitz cell (i.e. the Voronoi domain) and the primitive cell generate by translations the complexes $\mathscr{V}_\Gamma$ and $\mathscr{V}_\Gamma^*$ in the present notation, with the consequence that the two complexes are equivalent up to a translation. The Klotz construction for (hyper-)cubic lattices in dimensions $n = 2, 3, 6$ was introduced in [7]. The 'oblique' tilings introduced by Oguey *et al* [8] are essentially Klotz constructions for general hypercubic lattices. In [9] the concept of dual cell structures and related Klotz constructions for non-hypercubic lattices was proposed and illustrated for Bravais lattices in two dimensions and for centred cubic lattices in three dimensions. Here the dual complexes become inequivalent to one another.

The present approach based on Voronoi domains provides a new and very general framework for perfect and imperfect cell structures in quasicrystals. It has recently been applied to the four-dimensional root lattice A_4 and yields a new triangular tiling with pentagonal symmetry [10]. For the purpose of a theory of defects in quasicrystals, the next step would be an investigation of the effect of the whole variety of known dislocation scenarios in high-dimensional lattices on the ideal projected quasiperiodic patterns.

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