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Admissible Reversing and Extended Symmetries for Bijective Substitutions

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Abstract
In this paper, we deal with reversing and extended symmetries of subshifts generated by bijective substitutions. We survey some general algebraic and dynamical properties of these subshifts and recall known results regarding their symmetry groups. We provide equivalent conditions for a permutation on the alphabet to generate a reversing/extended symmetry, and algorithms how to compute them. Moreover, for any finite group H and any subgroup P of the d-dimensional hyperoctahedral group, we construct a bijective substitution which generates an aperiodic subshift with symmetry group $\mathbb{Z}^d \times H$ and extended symmetry group $(\mathbb{Z}^d \rtimes P) \times H$. A similar construction with the same symmetry group, but with extended symmetry group $(\mathbb{Z}^d \times H) \rtimes P$ is also provided under a mild assumption on the dimension.

Keywords Extended symmetries · Automorphism groups · Substitution subshifts · Aperiodic tilings

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1 Introduction

The study of symmetry groups, often also known as automorphism groups, is an important part of the analysis of a dynamical system, as it can offer insight on the behavior of the system, as well as allowing classifications of distinct families of dynamical systems (acting as a conjugacy invariant). In particular, symmetry groups of subshifts have been thoroughly studied (see e.g. the analysis of the symmetry group of the full shift [9], the series of works on symmetries in low-complexity subshifts [15–17], and recent works on shifts of algebraic and number-theoretic origin [3,19]).

Symmetries of subshifts can be algebraically defined as elements of the topological centralizer of the group $\langle\sigma\rangle$ generated by the shift, seen as a subgroup of the space $\mathrm{Aut}(\mathbb{X})$ of all self-homeomorphisms of $\mathbb{X}$ onto itself. Thus, a natural question at this point is whether the corresponding normalizer has an interesting dynamical interpretation as well. This leads to the concept of *reversing symmetries* (for $d=1$); see [5,6,23], the monograph [33] for a group-theoretic exposition, and [28] for a more physical background. These are special types of flip conjugacies; see [8]. In higher dimensions, one talks of *extended symmetries*; see [1,6], which are examples of $\mathrm{GL}(d,\mathbb{Z})$-conjugacies; compare [3,27]. These kinds of maps are related to phenomena such as palindromicity and several properties of geometric and topological nature, with the latter being more evident in the higher-dimensional setting [6,10].

High complexity is often (but not always, see for instance the square-free subshift [3]) linked to a complicated symmetry group. For instance, determining whether the symmetry groups of the full shifts in two and three symbols are isomorphic has consistently proven to be a difficult question [9]. The low-complexity situation, thus, often allows for a more in-depth analysis and more complete descriptions, up to and including explicit computation of these groups in many cases.

The particular case of substitutive subshifts has gathered significant attention and here a lot of progress has been made; see [26,32]. Unsurprisingly, the presence of non-trivial symmetries is also tied to the spectral structure of the underlying dynamical system; see [21,34]. In this work, we restrict to systems generated by bijective substitutions, both in one and in higher dimensions. These substitutions are typically n-to-1 extensions of odometers and generate colored tilings of $\mathbb{Z}^d$ by unit cubes, where one usually identifies a letter with a unique color; see [21]. Some natural questions in this direction are:

– What kinds of groups can appear as symmetry groups/extended symmetry groups of specific substitutive subshifts?
– Given a specific group H, can we construct a substitution whose associated subshift has H as its symmetry group/extended symmetry group?

Both questions are accessible for bijective substitutions. For symmetry groups, the second question is answered in full in [17], which extends to higher dimensions with no additional assumptions; see [13] for realization results for more general group actions.

The paper is organized as follows: In Sect. 2.1 we discuss the general properties of bijective substitution subshifts, which is followed by a discussion on their associated symmetry groups in Sect. 2.2. While most results in this section are known, we present them for completeness and to provide an overview regarding symmetry groups for this subclass. The reader may jump back and forth between Sects. 2.2 and 3 to compare both symmetry groups, where the extended one is now heavily dependent on the geometry of the supertiles and the relative positions of the permutations within the supertiles. This not only motivates the main results in Sect. 3, but also presents general structures which might be of independent interest apart from the study of symmetry groups. In particular, subshifts generated by bijective substitutions also provide good examples for studying other dynamical, combinatorial and spectral properties; see [7,26,34] for works on the Ellis semigroup, the dynamical spectrum and arithmetic progressions. It is conjectured that the dynamical spectrum of primitive bijective substitutions is purely singular, but the case when the group generated by the columns is non-abelian remains open [7].

We also provide an algorithm on how to compute the symmetry group given the substitution, where it is made apparent that the geometry *does not* play any role in determining the symmetry group; see Algorithm 1.

The main results of the paper concern extended symmetries and we develop them in Sect. 3. We deal with the one-dimensional case in Sect. 3.1. In Theorem 3.5, we provide equivalent conditions for the existence of reversing symmetries, and an algorithm which allows one to check whether such exist given a specific substitution; see Algorithm 2. We extend the analysis in higher dimensions in Sect. 3.2, where we generalize Theorem 3.5 in Theorem 3.13 to cover extended symmetries. We also provide sufficient conditions to rule out certain extended symmetries in Theorem 3.11.

As a corollary of Theorem 3.13, given any dimension d, a finite group H, and a subgroup P of the hyperoctahedral group P, we provide a construction in Theorem 3.18 of a bijective substitution whose subshift has symmetry group and extended symmetry group $\mathbb{Z}^d \times H$ and $(\mathbb{Z}^d \rtimes P) \times H$, respectively. A similar construction, with a different structure for the extended symmetry group, is done in Theorem 3.25.

2 Bijective Constant-Length Substitutions

2.1 Setting and Basic Properties

Let $\mathcal{A}$ be a finite alphabet and $\mathcal{A}^+ = \bigcup_{L\geq 1} \mathcal{A}^L$ be the set of finite non-empty words over $\mathcal{A}$; we shall write $\mathcal{A}^* = \mathcal{A}^+ \cup \{\varepsilon\}$, where the latter is the empty word. A *substitution* is a map $\varrho\colon \mathcal{A} \to \mathcal{A}^+$. If there exists an $L \in \mathbb{N}$ such that $\varrho(a) \in \mathcal{A}^L$ for all $a \in \mathcal{A}$, ϱ is called a *constant-length* substitution. Substitutions may be extended to arbitrary words from $\mathcal{A}^*$ by concatenation: for $u, v \in \mathcal{A}^*$, we have $\varrho(uv) := \varrho(u)\varrho(v)$. This allows one to define powers of ϱ inductively via $\varrho^k(a) := \varrho^{k-1}(\varrho(a))$ for $k \geq 2$. If there exists a power k such that $\varrho^k(a)$ contains all letters in $\mathcal{A}$, for every $a \in \mathcal{A}$, we call ϱ *primitive*.

The *full shift* is the set $\mathcal{A}^{\mathbb{Z}}$ of all functions (*configurations*) $x\colon \mathbb{Z} \to \mathcal{A}$. More generally, we define the d-dimensional full shift as the set $\mathcal{A}^{\mathbb{Z}^d}$. To this space, we assign the product topology, giving $\mathcal{A}$ the discrete topology. This is a particular version of the *local topology* used in tiling spaces and discrete point sets, in which two tilings (or point sets) x and y are said to be *ε-close* if a small translation of x (of magnitude less than ε) matches y on a large ball (of radius at least $1/\varepsilon$) around the origin; this can be used to define a metric $\mathrm{d}(x, y)$. In the particular case of subshifts seen as tiling spaces, since tiles are aligned with $\mathbb{Z}^d$, we can disregard the translation and get, e.g., the following as an equivalent metric:

$$\mathrm{d}(x, y) = 2^{-\inf\{n : x|_{[-n,n]^d} \neq y|_{[-n,n]^d}\}}.$$

This space is endowed with the *shift action* of $\mathbb{Z}^d$ on $\mathcal{A}^{\mathbb{Z}^d}$, which is the action of $\mathbb{Z}^d$ over configurations by translation, and can be defined via the equality $(\sigma_{\boldsymbol{n}}(x))_{\boldsymbol{m}} = x_{\boldsymbol{n}+\boldsymbol{m}}$ for all $x \in \mathcal{A}^{\mathbb{Z}^d}$, $\boldsymbol{m}, \boldsymbol{n} \in \mathbb{Z}^d$ (in particular, in one dimension we have the shift map $\sigma = \sigma_1$, which completely determines the group action).

A *subshift* is a topologically closed subset $\mathbb{X} \subseteq \mathcal{A}^{\mathbb{Z}^d}$ which is also invariant under the shift action. Thus, a subshift combined with the restriction of this group action to $\mathbb{X}$ defines a topological dynamical system, which can be endowed with one or more measures to obtain a measurable dynamical system. In the one-dimensional case, the *language* (or *dictionary*) of a subshift $\mathbb{X}$ is the set of all words that may appear in some $x \in \mathbb{X}$, that is:

$$\mathcal{L}(\mathbb{X}) = \{x|_{[0,n]} : x \in \mathbb{X},\ n \geq 0\} \cup \{\varepsilon\}.$$

We may verify that any non-empty set of words $\mathcal{L}$ which is *extensible* (that is, any $w \in \mathcal{L}$ is a subword of a longer word $uwv \in \mathcal{L}$, with u, v non-empty), and closed under taking subwords is the language of a subshift, and two subshifts are equal if and only if they share the same language.

Higher-dimensional subshifts have a similar combinatorial characterization, where the role of words is taken by *patterns*, that is, finite configurations of the form $P\colon U \subset \mathbb{Z}^d \to \mathcal{A}$, $|U| < \infty$; we identify a pattern with any of its translations. In most cases[1] (and, in particular, in the rest of this work), it makes no difference to allow arbitrary "shapes" U or to restrict ourselves to only rectangular patterns, i.e., products of intervals of the form $U = \prod_{i=1}^{d}[0, n_i - 1]$. Regardless of our chosen convention, we collect all valid patterns $x|_U$ that appear in some $x \in \mathbb{X}$ into a set $\mathcal{L}(\mathbb{X})$ as above, which we once again call the *language* of $\mathbb{X}$. As in the one-dimensional case, a language closed under taking subpatterns and where every pattern of shape U is contained in a pattern of shape $V \supset U$ for any larger (finite) V defines a unique subshift, and vice versa.

Thus, given that iterating a primitive substitution $\varrho\colon \mathcal{A} \to \mathcal{A}^L$ of constant length $L > 1$ over a symbol $a \in \mathcal{A}$ produces words of increasing length, the set $\mathcal{L}_\varrho$ of all words that are subwords of some $\varrho^k(a)$ for some $k \geq 1$ and $a \in \mathcal{A}$ is the language of a unique subshift that depends only on ϱ, which we shall call the *substitutive subshift* defined by ϱ and denote by $\mathbb{X}_\varrho$. This definition extends to d-dimensional

[1] Pattern shapes do matter when studying certain generalizations of topological mixing in the d-dimensional setting, where either restricting ourselves to specific shapes (rectangles, L-shapes, hollow rectangles, etc.) or allowing arbitrary ones may be preferable depending on context. However, we are not concerned with these kinds of properties here.

rectangular substitutions $\varrho\colon \mathcal{A} \to \mathcal{A}^R$ (where R is a product of intervals), which are higher-dimensional analogues of constant-length substitutions; see [7,21,34]. It is well known that the primitivity of ϱ implies that $\mathbb{X}_\varrho$ is strictly ergodic (uniquely ergodic and minimal); see [4,34]. We refer the reader to [31] for a treatment of substitutions which are non-primitive.

Definition 2.1 A constant-length substitution $\varrho\colon \mathcal{A} \to \mathcal{A}^L$ is called *bijective* if the map which is given by $\varrho_j : a \mapsto \varrho(a)_j$ is a bijection on $\mathcal{A}$, for all indices $0 \le j \le L-1$. Equivalently, ϱ is bijective if there exist L (not necessarily distinct) bijections $\varrho_0, \ldots, \varrho_{L-1}\colon \mathcal{A} \to \mathcal{A}$ such that $\varrho(a) = \varrho_0(a) \ldots \varrho_{L-1}(a)$ for every $a \in \mathcal{A}$. We shall refer to the mapping ϱ_j as the j-th *column* of the substitution ϱ.

Consider $\{\varrho_j\}_{j=0}^{L-1} \subset S_{|\mathcal{A}|}$. Let $\Phi\colon S_{|\mathcal{A}|} \to \mathrm{GL}(|\mathcal{A}|, \mathbb{Z})$ be the representation via permutation matrices. One then has the following; compare [21, Cor. 1.2].

Fact 2.2 *Let ϱ be a primitive, bijective substitution, whose columns are given by $\{\varrho_0, \ldots, \varrho_{L-1}\}$. Then the substitution matrix M is given by $M = \sum_{j=0}^{L-1} \Phi(\varrho_j^{-1})$. Moreover, $(1, 1, \ldots, 1)^T$ is a right Perron–Frobenius eigenvector of M, so each letter has the same frequency for every element in the subshift $\mathbb{X}_\varrho$, i.e., $\nu_a = 1/|\mathcal{A}|$ for all $a \in \mathcal{A}$ and all $x \in \mathbb{X}_\varrho$.*

Define the *n-th column group* $G^{(n)}$ to be the following subgroup of the symmetric group of bijections $\mathcal{A} \to \mathcal{A}$:

$$G^{(n)} := \bigl\langle \bigl\{ \varrho_{j_1} \circ \cdots \circ \varrho_{j_n} : 0 \le j_1, \ldots, j_n \le L-1 \bigr\} \bigr\rangle.$$

As it turns out, the groups $G^{(n)}$ generated by the columns give a good description of the substitution ϱ in the bijective case; see [26] for its relation to the corresponding Ellis semigroup of $\mathbb{X}_\varrho$. The primitivity of ϱ may be characterized entirely by this family of groups, as seen below. Recall that a subgroup $G \le S_n$ of the symmetric group on $\{1, \ldots, n\}$ is *transitive* if for all $1 \le j, k \le n$ there exists $\tau \in G$ such that $\tau(j) = k$. Here, we let $N \in \mathbb{N}$ be the minimal power such that $\varrho_j^N = \mathrm{id}$ for some $0 \le j \le L^N - 1$; compare [34, Lem. 8.1]. In [26], $G^{(N)}$ is called the *structure group* of ϱ.

Proposition 2.3 *Let $\varrho\colon \mathcal{A} \to \mathcal{A}^L$ be a bijective substitution. Then, the following are equivalent:*

(i) *The substitution ϱ is primitive.*
(ii) *All groups $G^{(n)}$, $n \in \mathbb{N}$, are transitive.*
(iiii) *The group $G^{(N)}$ is transitive.*

Proof Evidently, (ii) ⇒ (iii), so we only need to prove (iii) ⇒ (i) ⇒ (ii). To see the first implication, note first that the columns of the iterated substitution ϱ^N are compositions of the form $\varrho_{j_1,\ldots,j_N} := \varrho_{j_1} \circ \cdots \circ \varrho_{j_N}$, $0 \le j_1, \ldots, j_N \le L-1$, that is, for any $a \in \mathcal{A}$ the following holds:

$$\varrho^N(a) = \varrho_{0,\ldots,0,0}(a)\varrho_{0,\ldots,0,1}(a) \ldots \varrho_{0,\ldots,0,L-1}(a)\varrho_{0,\ldots,1,0}(a) \ldots \varrho_{L-1,\ldots,L-1,L-1}(a).$$

Since, by (iii), the group $G^{(N)}$ is transitive, the substitution matrix M_{ϱ^N} is irreducible, i.e., it is the adjacency matrix of a strongly connected directed graph. In other words, for all $a, b \in \mathcal{A}$, there exists a composition of columns $q, q', \ldots, q''$ of ϱ^N such that $q \circ q' \circ \cdots \circ q''(a) = b$, which may be identified with a path in the graph whose vertices are the letters of $\mathcal{A}$ and with one edge from c to $r(c)$ for any $c \in \mathcal{A}$ and column r. The choice of N also shows that M_{ϱ^N} has a non-zero diagonal, since one of the columns of ϱ^N is the identity. These two conditions immediately imply that M_{ϱ^N} is a primitive matrix (see [30, Chap. 2]) which in turn implies primitivity of ϱ, as desired.

To prove (i) $\Rightarrow$ (ii), note that primitivity of ϱ implies that, for some $k > 0$ and for all $a \in \mathcal{A}$, the word $\varrho^k(a)$ contains all symbols of the alphabet $\mathcal{A}$, including a itself. Since the columns of ϱ^k generate $G^{(k)}$, this implies that for all $a, b \in \mathcal{A}$ there is some generator of this group that maps a to b, i.e., $G^{(k)}$ is transitive. Since $\varrho^k(a)$ contains a as a subword, this implies that $\varrho^{2k}(a)$ contains $\varrho^k(a)$ as a subword, and, by induction, that $\varrho^{mk}(a)$ contains $\varrho^k(a)$ as a subword for all $m \geq 1$; thus, all groups $G^{(mk)}$ are transitive. Now, it is easy to see that $G^{(n)} \leq G^{(d)}$ if $d \mid n$. Then, for all $n \in \mathbb{N}$, $G^{(n)}$ has $G^{(nk)}$ as a transitive subgroup and hence it is transitive. □

The bijective structure of ϱ can also be exploited to conclude the aperiodicity of $\mathbb{X}_\varrho$ by just looking at simple features of ϱ. In the next result, we provide a criterion for aperiodicity in terms of $|\mathcal{A}|, L$.

Proposition 2.4 *Let $\mathbb{X}_\varrho$ be the subshift of a primitive, bijective substitution ϱ of length L on a finite alphabet $\mathcal{A}$. If* $\gcd(|\mathcal{A}|, L) > 1$ *then $\mathbb{X}_\varrho$ is aperiodic.*

Proof Assume that w^∞ is a periodic word in $\mathbb{X}_\varrho$ with least period p, i.e., $w^\infty = v^\infty$ with v being a prime period ($|v| = p$). Then without loss of generality, we assume that w^∞ is fixed under ϱ by replacing it with a power ϱ^k such that the first column of ϱ^k is the identity. We choose the smallest possible constants $c, d \in \mathbb{N}$ which satisfy $cL = dp$. That is, the word $w^\infty|_{[0,cL-1]}$ is an inflation of c letters and, at the same time, d copies of the prime period. Since ϱ is a bijective substitution of length L, every inflation word of length cL has exactly one preimage under ϱ, which is a word of length c. In particular, since w^∞ is fixed under ϱ, the preimage of $w^\infty|_{[0,cL-1]}$ under ϱ must be an initial segment $x_1 \ldots x_c$ of w^∞ of length c. As cL is a multiple of p, then, for any $k \in \mathbb{Z}$, $w^\infty|_{[0,cL-1]} = (\sigma^{kcL}(w^\infty))_{[0,cL-1]}$, which all have the same preimage under ϱ. This means that w^∞ is an infinite concatenation of copies of $x_1 \ldots x_c$ and is thus c-periodic. As p is the least period, we must have $c = ep$ for some integer e. Since c is minimal $c = p$ and thus $d = L$, which certainly solves $cL = dp$.

From Fact 2.2 we know that every letter has the same frequency for any element in $\mathbb{X}_\varrho$. This, together with the fact that w^∞ is a concatenation of v, implies that every letter appears equally often within v, so $|\mathcal{A}| \mid p$. If $\gcd(|\mathcal{A}|, L) > 1$ then $\gcd(p, L) = a > 1$ as well. But then $cL/a = dp/a$ holds and $c' = c/a$ and $d' = d/a$ are smaller integer constants contradicting the minimality of c and d. So our assumption that w^∞ is periodic has to be false. □

Another way to get aperiodicity is through the existence of proximal pairs; see [17, Sect. 3.2.1] and [4, Cor. 4.2 and Thm. 5.1]. Two elements $x \neq y \in (\mathbb{X}, \sigma)$ are said to be proximal if there exists a subsequence $\{n_k\}$ of $\mathbb{N}$ or $-\mathbb{N}$ such that $\mathrm{d}(\sigma^{n_k}x, \sigma^{n_k}y) \to 0$ as

$k \to \infty$. A stronger notion is that of asymptoticity, which requires $\mathrm{d}(\sigma^n x, \sigma^n y) \to 0$ as $n \to \infty$ or $-\infty$. For bijective substitutions, these two notions are equivalent, and asymptotic pairs are completely characterized by fixed points of ϱ. The following is an equivalent condition for aperiodicity in terms of existence of certain legal words; see [26].

Proposition 2.5 [26, Prop. 4.1] *Let ϱ be a primitive, bijective substitution on a finite alphabet $\mathcal{A}$ in one dimension. Then the subshift $\mathbb{X}_\varrho$ is aperiodic if and only if there exist distinct legal words of length 2 which either share the same starting or ending letter.*

Example 2.6 The substitution $\varrho\colon a \mapsto aba, b \mapsto bab$ is primitive, bijective and admits a periodic subshift. Here, the only legal words of length 2 are ab and ba. Note that ϱ generates the same subshift as the substitution $\varrho'\colon a, b \mapsto ab$.

2.2 Symmetries

In the following sections, we deal with the *symmetry groups* of our subshifts of interest, which are certain homeomorphisms of the subshift which preserve the dynamics of the shift action in a specific sense.

Definition 2.7 Let $\mathbb{X}$ be a $\mathbb{Z}^d$-subshift. The *symmetry group* (often called *automorphism group*[2]) is the set $\mathcal{S}(\mathbb{X})$ of all homeomorphisms $\mathbb{X} \to \mathbb{X}$ which commute with the shift action, i.e.,

$$(\forall\, \boldsymbol{n} \in \mathbb{Z}^d)\colon\ \sigma_{\boldsymbol{n}} \circ f = f \circ \sigma_{\boldsymbol{n}}. \tag{1}$$

That is, $\mathcal{S}(\mathbb{X})$ is the centralizer of the set of shift maps in the group of all self-homeomorphisms of the space $\mathbb{X}$. In this context, every symmetry $f \in \mathcal{S}(\mathbb{X})$ is entirely determined by a *local function*, a mapping $F\colon \mathcal{A}^U \to \mathcal{A}$, with $U \subset \mathbb{Z}^d$ finite, such that for every $\boldsymbol{n} \in \mathbb{Z}^d$, $f(x)_{\boldsymbol{n}} = F(x|_{\boldsymbol{n}+U})$. This fact is known as the *Curtis–Hedlund–Lyndon (or CHL) theorem*; see [30] for the formulation in one dimension and [11, Thm. 1.8.1] for the general setting where $\mathcal{A}^G$ is the full shift, G being a general group. We say that f has *radius* $r \geq 0$ if this is the least non-negative integer for which we may find $U \subseteq [-r, r]^d$.

Symmetry groups of one-dimensional bijective substitutions are a thoroughly studied subject, both in the topological and ergodic-theoretical contexts. Complete characterizations of these groups are known, as seen in e.g. [14] for a two-symbol alphabet, or [29] for a characterization in the measurable case; see also [15,21] for further elaboration in the description of the symmetries in this category of subshifts. The following theorem summarizes this classification:

Theorem 2.8 *Let $\mathbb{X}_\varrho$ be the subshift generated by an aperiodic, primitive, bijective substitution ϱ on $\mathbb{Z}^d$. Then, the symmetry group $\mathcal{S}(\mathbb{X}_\varrho)$ is isomorphic to the direct product of $\mathbb{Z}^d$, generated by the shift action, with a finite group of radius-*0 *sliding*

[2] In this work, we follow the notational conventions of [6], and thus we avoid the term "automorphism group" as it may be understood as the set of all homeomorphisms $f\colon \mathbb{X} \to \mathbb{X}$.

block codes $\tau_\infty\colon \mathbb{X}_\varrho \to \mathbb{X}_\varrho$ *given by* $\tau_\infty((x_{\boldsymbol{j}})_{\boldsymbol{j}\in\mathbb{Z}^d}) = (\tau(x_{\boldsymbol{j}}))_{\boldsymbol{j}\in\mathbb{Z}^d}$ *for some bijection* $\tau\colon \mathcal{A} \to \mathcal{A}$. *Moreover, let* N *be any integer such that* $\varrho_{\boldsymbol{j}}^N$ *is the identity for some* $\boldsymbol{j}$ (*note that such an* N *always exists*). *Then,* $\tau\colon \mathcal{A} \to \mathcal{A}$ *induces a symmetry if and only if* $\tau \in \mathrm{cent}_{S_{|\mathcal{A}|}} G^{(N)}$.

As a consequence, every symmetry on $\mathbb{X}_\varrho$ is a composition of a shift map and a radius-0 sliding block code as above. These conditions arise as a consequence of such a symmetry having to preserve the supertile structure of any $x \in \mathbb{X}_\varrho$ at every scale, which in particular implies that a level-k supertile $\varrho^k(a)$, $a \in \mathcal{A}$, has to be mapped to some $\varrho^k(b)$ for some other $b \in \mathcal{A}$ by the "letter exchange map" τ. The choice of N above ensures that, when k is a multiple of N, the equality $a = b$ holds, which implies that τ commutes with the columns of ϱ^N, and thus $\varrho^N \circ \tau_\infty = \tau_\infty \circ \varrho^N$. This in turn implies (1). For further elaboration on the proof of the above result, the reader may consult [15,21], among others.

Example 2.9 Consider the following substitution ϱ on the three-letter alphabet $\mathcal{A} = \{a, b, c\}$:

$$\varrho\colon \quad a \mapsto abc,\ b \mapsto bca,\ c \mapsto cab.$$

The columns correspond to the three elements of the cyclic group generated by $\tau = (a\,b\,c)$. It is not hard to verify that the only elements of $S_3 = D_3$ that commute with τ are the powers of τ themselves, and thus $\mathcal{S}(\mathbb{X}_\varrho) \simeq \mathbb{Z} \times C_3$, with the finite subgroup C_3 being generated by the symmetries induced by the powers of τ.

As it turns out, Theorem 2.8 provides an algorithm to compute $\mathcal{S}(\mathbb{X}_\varrho)$ explicitly. To introduce this algorithm, let us recall some easily verifiable facts from group theory [24, Chaps. 1 and 5]:

Fact 2.10 *Let* G *be any group and* $H = \langle S\rangle \le G$ *be a subgroup generated by* $S \subset G$. *Then,*

$$\mathrm{cent}_G(H) = \{c \in G : (\forall\, h \in H)\colon ch = hc\} = \bigcap_{s\in S} \mathrm{cent}_G(s).$$

Fact 2.11 *Any permutation decomposes uniquely (up to reordering) as a product of disjoint cycles. Conjugation by some* $\tau \in S_n$ *can be computed from this decomposition using the identity:*

$$\tau(a_1\, a_2\, \ldots\, a_n)\tau^{-1} = (\tau(a_1)\tau(a_2)\ldots\tau(a_n)).$$

A permutation $\tau \in S_n$ *belongs to* $\mathrm{cent}_{S_n}(\pi)$ *if and only if* $\tau\pi\tau^{-1} = \pi$, *and thus:*

$$\begin{aligned}\pi &= (a_1a_2\ldots a_{k_1})(b_1b_2\ldots b_{k_2})\cdots(c_1c_2\ldots c_{k_r})\\ &= (\tau(a_1)\tau(a_2)\ldots\tau(a_{k_1}))(\tau(b_1)\tau(b_2)\ldots\tau(b_{k_2}))\cdots(\tau(c_1)\tau(c_2)\ldots\tau(c_{k_r})).\end{aligned}$$

Hence, the uniqueness of this decomposition implies that every cycle in the second decomposition is equal to a cycle of the same length in the first one.

Thus, to compute the letter exchange maps that determine $\mathcal{S}(\mathbb{X}_\varrho)$, we need to find all permutations τ that preserve certain cycle decompositions. From Facts 2.10 and 2.11, we obtain the following procedure:

Algorithm 1. Assuming that ϱ is a primitive, bijective, aperiodic substitution, the following algorithm computes $\mathcal{S}(\mathbb{X}_\varrho)$ explicitly.

- **Input:** ϱ is a length-L bijective substitution, which may be represented as a function (dictionary) $\varrho\colon \mathcal{A} \to \mathcal{A}^L$ or a set of L permutations $\varrho_0, \varrho_1, \ldots, \varrho_{L-1}\colon \mathcal{A} \to \mathcal{A}$, corresponding to each column.
- **Output:** A (finite) set of permutations C forming a group, so that $\mathcal{S}(\mathbb{X}_\varrho) = \mathbb{Z}^d \times H$.

(1) Compute the least positive integer N such that ϱ_j^N is the identity on $\mathcal{A}$ for some column of the substitution ϱ. N equals the least common multiple of all cycle lengths in the decomposition of the columns ϱ_j into disjoint cycles (and is thus finite).

(2) Determine all columns $\varrho_{j_1} \circ \cdots \circ \varrho_{j_N}$ of the iterated substitution ϱ^N. This is a generating set for the group $G^{(N)}$.

(3) For every column computed in (2), compute $G_{j_1,\ldots,j_N} = \mathrm{cent}_{S_n}(\varrho_{j_1} \circ \cdots \circ \varrho_{j_N})$ by taking the cycle decomposition of this permutation (in where we identify $\mathcal{A}$ with the set $\{1, 2, \ldots, |\mathcal{A}|\}$) and employing the characterization above.

(4) Let $H = \bigcap_{j_1,\ldots,j_n} G_{j_1,\ldots,j_N}$. As H can be biunivocally identified with the set of valid letter exchange maps modulo a shift, return $\mathcal{S}(\mathbb{X}_\varrho) = \mathbb{Z}^d \times H$ as output.

Example 2.9 above corresponds to a simple case in which $G^{(N)} = G^{(1)}$ is a cyclic group, and we derive an abelian subgroup of S_3 corresponding to the valid letter exchange maps. We can use the above procedure to construct examples with more complicated symmetry groups, see Example 2.12.

Example 2.12 We take as alphabet the *quaternion group* $Q_8 = \{e, i, j, k, \bar{e}, \bar{\imath}, \bar{\jmath}, \bar{k}\}$ (see [24] for the multiplication table and basic properties of this group, which is generated by the two elements i and j). With this, we construct a length-3 bijective substitution defined by right multiplication, $x \mapsto (x \cdot i)(x \cdot j)(x \cdot k)$, given in full by

$$\begin{array}{llll} e \mapsto ijk, & \bar{e} \mapsto \bar{\imath}\bar{\jmath}\bar{k}, & i \mapsto \bar{e}k\bar{\jmath}, & \bar{\imath} \mapsto e\bar{k}j, \\ j \mapsto \bar{k}\bar{e}i, & \bar{\jmath} \mapsto ke\bar{\imath}, & k \mapsto j\bar{\imath}\bar{e}, & \bar{k} \mapsto \bar{\jmath}ie. \end{array}$$

– The three permutations obtained from the columns which generate $G^{(1)}$ are

$$R_i := (e\, i\, \bar{e}\, \bar{\imath})(j\, \bar{k}\, \bar{\jmath}\, k), \qquad R_j := (e\, j\, \bar{e}\, \bar{\jmath})(i\, k\, \bar{\imath}\, \bar{k}), \qquad R_k := (e\, k\, \bar{e}\, \bar{k})(j\, i\, \bar{\jmath}\, \bar{\imath}).$$

Thus, the substitution ϱ^3 has as columns $R_{xyz}(g) = g \cdot xyz$ with $x, y, z \in \{i, j, k\}$; in particular, since $jik = e$, ϱ^3 must have an identity column.

– By direct computation, $G^{(n)} = G^{(1)} \simeq Q_8$ for all n, making the substitution primitive (as Q_8 acts transitively on itself in an obvious way). Also, since $G^{(3)} = G^{(1)}$, this group is the right Cayley embedding of Q_8 into S_8.

– By applying the above algorithm, we obtain that the group of letter exchange maps is generated by the following two permutations:

$$\pi_0 := (e\, i\, \bar{e}\, \bar{\imath})(j\, k\, \bar{\jmath}\, \bar{k}), \qquad \pi_1 := (e\, j\, \bar{e}\, \bar{\jmath})(i\, \bar{k}\, \bar{\imath}\, k).$$

We can verify that these permutations generate the *left* Cayley embedding of Q_8 into S_8. Alternatively, if we consider the transposition $\nu = (k\,\bar{k})$, we can use Fact 2.11 above to see that $\pi_0 = \nu R_i \nu^{-1}$ and $\pi_1 = \nu R_j \nu^{-1}$, which in turn implies that the group generated by π_0 and π_1 is conjugate to the group generated by R_i and R_j, the latter being isomorphic to Q_8. This shows that $\mathcal{S}(\mathbb{X}_\varrho) \simeq \mathbb{Z} \times Q_8$.

It is well known that symmetry groups of aperiodic minimal one-dimensional subshifts are virtually $\mathbb{Z}$. The following result gives a full converse for shifts generated by bijective substitutions.

Theorem 2.13 [17, Thm. 3.6] *For any finite group H, there exists an explicit primitive, bijective substitution ϱ, on an alphabet on $|H|$ letters, such that $\mathcal{S}(\mathbb{X}_\varrho) \simeq \mathbb{Z} \times H$.*

The proof, which may be consulted in [17], follows a similar schema to the analysis done in Example 2.12 above. In [21, Sect. 4.1], it was shown that the number of letters needed in Theorem 2.13 is actually a tight lower bound. Below, we actually prove something stronger.

Proposition 2.14 *Let ϱ be an aperiodic, primitive and bijective substitution on a finite alphabet $\mathcal{A}$. If $\mathcal{S}(\mathbb{X}_\varrho) \simeq \mathbb{Z} \times H$, then H must act freely on $\mathcal{A}$, and the order of H has to divide $|\mathcal{A}|$.*

Proof As seen in [21, Sect. 4.1], if we replace ϱ with a suitable power, we may ensure that the word $\varrho^q(a)$ starts with a and contains every other symbol, for all $a \in \mathcal{A}$. Thus, for any $\pi \in S_n$, the equality $\pi(a) = b$ implies $\pi(\varrho^q(a)) = \varrho^q(b)$, which in turn determines the images of every symbol in the alphabet; the bound $|H| \leq |\mathcal{A}|$ follows from here.

Note as well that, since ϱ is bijective, if $\pi(a) \neq a$, then $\pi(c) \neq c$ for every $c \in \mathcal{A}$ as the words $\varrho^q(a)$ and $\varrho^q(b)$ are either equal or differ at every position. This implies that if π has any fixed point then it must be the identity, i.e., that, if we identify H with the corresponding group of permutations over $\mathcal{A}$, the action of H on the alphabet is free. Equivalently, the stabilizer $\mathrm{Stab}(c)$ of any $c \in \mathcal{A}$ is the trivial subgroup.

The elements of H commute with every column of ϱ^q. Due to primitivity, there always exists a column $\varrho^* = \varrho_{j_1} \circ \cdots \circ \varrho_{j_q}$ which maps this a to any desired $c \in \mathcal{A}$. Since ϱ^* commutes with every $\pi \in H$ (i.e., it is an equivariant bijection for the action of H on $\mathcal{A}$), we have that $\mathrm{Orb}(c) = \varrho^*[\mathrm{Orb}(a)]$, i.e., the orbit of c under H is necessarily the image of the orbit of a under ϱ^*. Thus, every orbit is a set of the same cardinality. This means that H induces a partition of $\mathcal{A}$ into disjoint orbits of the same cardinality ℓ, which then must divide $|\mathcal{A}|$. By the freeness of the group action and the orbit-stabilizer theorem, $|H| = |\mathrm{Orb}(a)| \cdot |\mathrm{Stab}(a)| = \ell$, and thus $|H|$ divides $|\mathcal{A}|$. □

Remark 2.15 It follows from Theorem 2.14 that the substitution in Example 2.12 is a minimal one in the sense that for one to get a Q_8-extension in $\mathcal{S}(\mathbb{X}_\varrho)$, one needs at least eight letters.

Remark 2.16 At no point in the proof of Theorem 2.13 found in [17] nor in Theorem 2.14 above the fact that the substitution was one-dimensional is actually used. Thus, since Theorem 2.8 is known to be valid for general rectangular substitutions, the two theorems above must be valid in this more general setting as well, provided that the substitution is aperiodic in $\mathbb{Z}^d$, which one can always guarantee; see Propositions 2.5 and 3.16.

Corollary 2.17 *For any finite group H, there exists an explicit primitive, bijective d-dimensional rectangular substitution ϱ, on an alphabet of $|H|$ letters, such that $\mathcal{S}(\mathbb{X}_\varrho) \simeq \mathbb{Z}^d \times H$. Furthermore, this is the least possible alphabet size: for any bijective, primitive and aperiodic d-dimensional rectangular substitution ϱ on the alphabet $\mathcal{A}$, if $\mathcal{S}(\mathbb{X}_\varrho) \simeq \mathbb{Z}^d \times H$, then H acts freely on $\mathcal{A}$, and $|H|$ divides $|\mathcal{A}|$.*

3 Extended and Reversing Symmetries of Substitution Shifts

3.1 One-Dimensional Shifts

Since the term *symmetry group* does not cover everything that can be thought of as a symmetry (in the geometric sense of the word) we introduce the notion of the reversing symmetry group; see [6] for a detailed exposition. We will exclusively look at subshifts $\mathbb{X}_\varrho$ which are given by a bijective, primitive substitution ϱ and we will exploit this additional structure in determining the reversing symmetry group for this class.

Definition 3.1 The *extended symmetry group* of a subshift $\mathbb{X}$ is given as

$$\mathcal{R}(\mathbb{X}) := \mathrm{norm}_{\mathrm{Aut}(\mathbb{X})}(\mathcal{G}) = \{f \in \mathrm{Aut}(\mathbb{X}) : f\mathcal{G} = \mathcal{G}f\},$$

where $\mathcal{G}$ is the group generated by the shift action. In the case where the subshift is one-dimensional, we call $\mathcal{R}(\mathbb{X})$ the *reversing symmetry group* given by

$$\mathcal{R}(\mathbb{X}) = \{f \in \mathrm{Aut}(\mathbb{X}) : f \circ \sigma \circ f^{-1} = \sigma^{\pm 1}\}.$$

A homeomorphism $f \in \mathrm{Aut}(\mathbb{X})$ which satisfies $f \circ \sigma \circ f^{-1} = \sigma^{-1}$ is called a *reversor* or a *reversing symmetry*. A Curtis–Hedlund–Lyndon-type characterization of reversing symmetries, which incorporates the mirroring component ($\mathrm{GL}(d, \mathbb{Z})$-component in higher dimensions) can be found in [6].

In what follows, we investigate the effect of a reversor f on inflated words when one restricts to bijective substitutions. Given a substitution $\varrho\colon \mathcal{A} \to \mathcal{A}^L$, $\varrho := \varrho_0\varrho_1 \ldots \varrho_{L-1}$, the mirroring operation m acts on the columns of ϱ via $m(\varrho(a)) = \varrho_{L-1}(a) \ldots \varrho_2(a)\varrho_0(a)$. We may extend this to infinite configurations over $\mathbb{Z}$ in two non-equivalent ways, given by $m(x)_k = x_{-k}$ and $m'(x)_k = x_{1-k}$, respectively; we shall refer to both as basic mirroring maps.

Proposition 3.2 *Let ϱ be an aperiodic, primitive, bijective substitution. Then, any reversor is a composition of a letter exchange map $\pi \in S_n$, where $n = |\mathcal{A}|$, a shift map σ^k and one of the two basic mirroring maps m or m' (depending only on whether the substitution has odd or even length, respectively).*

Essentially, reversors are radius-0 maps except for the shift component; see [6, Prop. 1] and Theorem 2.8. This result, while desirable, is not immediately obvious (and can indeed be false for non-bijective substitutions, which may have reversors whose local

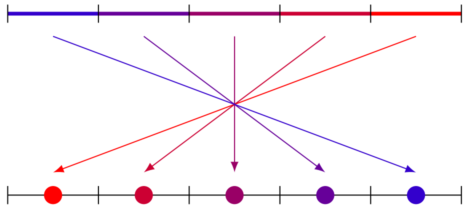


Fig. 1 A reversor f establishes a 1–1 correspondence between words $\varrho^k(a)$ in a point x and its image $f(x)$

functions have positive radius), and thus we show this result as a consequence of bijectivity.

Proof Suppose $f\colon \mathbb{X}_\varrho \to \mathbb{X}_\varrho$ is a reversor of positive radius $r \geq 1$, i.e., $x|_{[-r,r]} = y|_{[-r,r]}$ implies that one has $f(x)_0 = f(y)_0$. There is some power $k \geq 1$ such that the words $\varrho^k(a)$ of length L^k are longer than the local window of f, which has length $2r+1$ (say, $k = \lceil \log(2r+1)/\log L \rceil$). Any point of $\mathbb{X}_\varrho$ is a concatenation of words of the form $\varrho^k(a)$, $a \in \mathcal{A}$, which is unique up to a shift because of aperiodicity; see [37]. In particular, if we choose a fixed $x \in \mathbb{X}_\varrho$ and let $y = f(x)$, both points have such a decomposition.

Now, suppose that the value $L^k = 2\ell+1$ is odd (the case where L is even is dealt with similarly). By composing f with an appropriate shift map (say $\tilde{f} = f \circ \sigma^h$), we can ensure that the central word $\varrho^k(a)$ in the aforementioned decomposition has support $[-\ell, \ell]$ for both x and y (note that we employ the uniqueness of the decomposition here, to avoid ambiguity in the chosen h). Since $L^k = 2\ell + 1 \geq 2r + 1$, we must have $\ell \geq r$, and thus y_0 is entirely determined by $x|_{[-\ell,\ell]}$, which is a substitutive word $\varrho^k(a)$; see Fig. 1. But, since ϱ is bijective, this word is in turn completely determined by its central symbol x_0.

A similar argument shows that, for any $n \in \mathbb{Z}$, if $n \in mL^k + [-\ell, \ell]$, then y_n depends only on the word $x|_{-mL^k+[-\ell,\ell]}$, which contains (and is thus entirely determined by) x_{-n}. Since any point in $\mathbb{X}_\varrho$ is transitive, $\tilde{f}$ is entirely determined by the points x and y, and thus, $\tilde{f}$ is a map of radius 0. Equivalently, for some bijection $\pi\colon \mathcal{A} \to \mathcal{A}$, we have $\tilde{f}(x)_{-n} = \pi(x_n)$, that is, $\tilde{f} = f \circ \sigma^h = \pi \circ m$ (identifying π with the letter exchange map $\mathcal{A}^\mathbb{Z} \to \mathcal{A}^\mathbb{Z}$). We conclude that f is a composition of a letter exchange map, a mirroring map and a shift map. □

Remark 3.3 With some care, it can be shown that the same argument applies in the higher-dimensional case, where an element of the normalizer is a composition of a letter exchange map, a map of the form $f(x)_{\boldsymbol{n}} = x_{A\boldsymbol{n}}$, with A a linear map from the hyperoctahedral group (see Theorem 3.9), and a shift map; see [6, Prop. 3] for a more general formulation.

This result leads to the following criterion for the existence of a reversor in terms of the columns ϱ_i.

Proposition 3.4 *Let ϱ be an aperiodic, primitive and bijective substitution ϱ of length L on a finite alphabet $\mathcal{A}$ of n letters. Suppose that there exists a letter-exchange map*

$\pi \in S_n$, $\pi : \mathcal{A} \to \mathcal{A}$, which gives rise to a reversing symmetry. Then one has

$$\pi^{-1} \circ \varrho_i \circ \varrho_j^{-1} \circ \pi = \varrho_{L-(i+1)} \circ \varrho_{L-(j+1)}^{-1} \tag{2}$$

for all $0 \le i, j \le L-1$, where ϱ_i is the ith column of ϱ seen as an element of S_n.

Proof Let $a \in \mathcal{A}$. Let m be the mirroring operation and suppose that there exists $\pi \in S_n$ such that $m \circ \pi$ extends to a reversor $f \in \mathcal{R}(\mathbb{X}_\varrho)$. One then has

$$\varrho(a) = \varrho_0(a) \ldots \varrho_{L-1}(a) \xmapsto{m} \varrho_{L-1}(a) \ldots \varrho_0(a) \xmapsto{\pi} \pi \circ \varrho_{L-1}(a) \ldots \pi \circ \varrho_0(a).$$

Since Proposition 3.2 guarantees that this must result in mapping substituted words to substituted words, one gets

$$\pi \circ \varrho_{L-1}(a) \ldots \pi \circ \varrho_0(a) = \varrho_0(b) \ldots \varrho_{L-1}(b) = \varrho_0 \circ \tau(a) \ldots \varrho_{L-1} \circ \tau(a), \tag{3}$$

where the permutation τ describes precisely this induced shuffling of inflation words. This yields

$$\tau = \varrho_j^{-1} \circ \pi \circ \varrho_{L-(j+1)}$$

for all $0 \le j \le L-1$. Equating the corresponding right hand-sides for some pair i, j yields (2). The claim follows since this must hold for all $0 \le i, j \le L-1$. $\square$

Theorem 3.5 *Let ϱ be as in Proposition 3.4. Suppose further that $\varrho_i = \varrho_{L-(i+1)} = \mathrm{id}$ for some $0 \le i \le L-1$. Then, given a permutation (letter exchange map) $\pi \in S_n$, $\pi : \mathcal{A} \to \mathcal{A}$, the following are equivalent:*

(i) *The letter exchange map π gives rise to a reversing symmetry $f \in \mathcal{R}(\mathbb{X}_\varrho) \backslash \mathcal{S}(\mathbb{X}_\varrho)$ given by either $f(x)_n = \pi(x_{-n})$ or $f(x)_n = \pi(x_{1-n})$.*

(ii) *The permutation π satisfies the system of equations*

$$\pi^{-1} \circ \varrho_i \circ \pi = \varrho_{L-(i+1)} \tag{4}$$

for all $0 \le i \le L-1$.

(iii) *There exist $\kappa_0, \kappa_1, \ldots, \kappa_{L-1} \in S_n$, where each κ_i satisfies $\kappa_i^{-1} \circ \varrho_i \circ \kappa_i = \varrho_{L-(i+1)}$, such that the following intersection of cosets is non-empty:*

$$K = \bigcap_{i=0}^{L-1} \mathrm{cent}_{S_n}(\varrho_i)\kappa_i, \tag{5}$$

and $\pi \in K$.

Proof It is clear that (4) implies (2). Note that it is sufficient to satisfy (2) for $j = i+1 \mod L$ as any term can be obtained by multiplying sufficient numbers of succeeding terms. Under the extra assumption that there exist a column pair which is the identity, (2) simplifies to (4). This shows that (i) $\Rightarrow$ (ii).

For the other direction, we show that if (4) is satisfied by the level-1 inflation words, then these sets of equations must also be fulfilled by any power ϱ^k of ϱ. Remember that, from any arbitrary bijective substitution ϱ, we may derive another bijective substitution ϱ' that satisfies the additional condition of having two identity columns in opposing positions by choosing $k = \operatorname{lcm}(|\varrho_0|, |\varrho_{L-1}|)$ and replacing ϱ by its kth power, $\varrho' := \varrho^k$. This makes no difference when studying $\mathcal{R}(\mathbb{X}_\varrho)$, because ϱ and ϱ^k define the same subshift and the group of reversing symmetries is a property of the subshift.

First, we prove an important property of the columns of powers. Fix a power $k \in \mathbb{N}$ and pick a column ϱ_i of ϱ^k, where $0 \le i \le L^k - 1$. One then has $\varrho_i = \varrho_{i_0} \dots \varrho_{i_{k-1}}$ where $i_0 i_1 \dots i_{k-1}$ is the L-adic expansion of i and ϱ_{i_ℓ} are columns of the level-1 substitution ϱ.

The corresponding L-adic expansion of $L^k - (i+1)$ is then given by

$$L^k - (i+1) = (L - (i_0 + 1)) \dots (L - (i_{k-1} + 1)).$$

This can easily be shown via the following direct computation:

$$\sum_{j=0}^{k-1} (L - (i_j + 1)) L^j = \sum_{j=0}^{k-1} (L^{j+1} - L^j) - \sum_{j=0}^{k-1} i_j L^j = L^k - (i+1).$$

This implies that if one considers the corresponding column $\varrho_{L^k-(i+1)}$ one gets that

$$\varrho_{L^k-(i+1)} = \varrho_{L-(i_0+1)} \dots \varrho_{L-(i_{k-1}+1)}. \tag{6}$$

This has two consequences. First, if ϱ has an identity column pair, then all powers of ϱ admit at least one identity column pair. For each power k one just needs to choose ϱ_j with $j = ii \dots i$, which implies $\varrho_j = \varrho_i^k = \mathrm{id}$. By (6), we also get that $\varrho_{L^k-(j+1)} = (\varrho_{L-(i+1)})^k = \mathrm{id}$. In fact, ϱ^k contains at least 2^{k-1} pairs of identity columns.

Second, this property allows one to prove that if ϱ satisfies the system of equations in (4), then it is satisfied at all levels, i.e., by all powers of ϱ. To this end, choose $0 \le i \le L^k - 1$ with L-adic expansion $i_0 i_1 \dots i_{k-1}$. From (4) one then obtains

$$\begin{aligned}\pi^{-1} \circ \varrho_i \circ \pi &= \pi^{-1} \circ \varrho_{i_0} \dots \varrho_{i_{k-1}} \circ \pi = \pi^{-1} \varrho_{i_0} \pi \pi^{-1} \dots \pi \pi^{-1} \varrho_{i_{k-1}} \pi \\ &= \varrho_{L-(i_0+1)} \dots \varrho_{L-(i_{k-1}+1)} = \varrho_{L^k-(i+1)}.\end{aligned}$$

Since i is chosen arbitrarily and π induces a permutation of the substituted words at all levels, this means it extends to a map $f = \sigma_n \circ m \circ \pi \colon \mathbb{X}_\varrho \to \mathbb{X}_\varrho$, which by Proposition 3.2 is a reversor. This shows (ii) ⇒ (i).

To prove the remaining equivalences, note that if $\pi_1, \pi_2 \in S_n$ are two permutations satisfying the equality $\pi^{-1} \circ \varrho_i \circ \pi = \varrho_{L-(i+1)}$, then we have

$$\pi_1 \circ \varrho_{L-(i+1)} \circ \pi_1^{-1} = \varrho_i \quad \Longrightarrow \quad (\pi_2 \circ \pi_1^{-1})^{-1} \circ \varrho_i \circ (\pi_2 \circ \pi_1^{-1}) = \varrho_i,$$

that is, $(\pi_2 \circ \pi_1^{-1}) \in \mathrm{cent}_{S_n}(\varrho_i)$. As a consequence, π_1 belongs to the right coset $\mathrm{cent}_{S_n}(\varrho_i)\pi_2$ for any choice of π_1, π_2, and, since right cosets are either equal or disjoint, this means that all solutions of (4), for a fixed i, lie in the same right coset of $\mathrm{cent}_{S_n}(\varrho_i)$. Reciprocally, if π satisfies (4) and $\gamma \in \mathrm{cent}_{S_n}(\varrho_i)$, it is easy to verify that $\gamma \circ \pi$ satisfies (4) as well. Thus, the set of solutions of this equation is either empty or the aforementioned uniquely defined right coset.

Thus, suppose that π satisfies (4) for all $0 \le i \le L-1$. The set of solutions for each i equals the unique coset $\mathrm{cent}_{S_n}(\varrho_i)\pi$, and thus the set of all permutations that satisfy (4) for all i is exactly the intersection of all these cosets, i.e., $\bigcap_{i=0}^{L-1} \mathrm{cent}_{S_n}(\varrho_i)\pi$. Taking $\kappa_i = \pi$ for all i, we see that this is exactly the set K from (5). Evidently, π belongs to this intersection, and so we conclude that (ii) $\Rightarrow$ (iii).

As stated before, our choice of κ_i ensures that the set $\mathrm{cent}_{S_n}(\varrho_i)\kappa_i$ is exactly the set of solutions of (4) for a given i; thus, any permutation π that satisfies all of these equalities must be in all of these cosets and thus in the intersection (5), which is therefore non-empty. This shows that (iii) $\Rightarrow$ (ii), concluding the proof. $\square$

Remark 3.6 It is a known fact from group theory that, if $g_1, \ldots, g_r$ are elements of a group G and $H_1, \ldots, H_r$ are subgroups of this group, the intersection of cosets $\bigcap_{i=1}^{r} g_i H_i$ is either empty or a coset of $\bigcap_{i=1}^{r} H_i$. In this case, the latter intersection is exactly the group of non-trivial standard symmetries modulo a shift (letter exchanges), and thus, if there exist non-trivial reversing symmetries, these must all belong to a single coset of the group of valid letter exchanges. This is consistent with the fact that $\mathcal{R}(\mathbb{X}_\varrho)$ is at most an index 2 group extension of $\mathcal{S}(\mathbb{X}_\varrho)$ (in the 1-dimensional case).

Item (iii) in Theorem 3.5 provides an explicit algorithm to compute the group of permutations π which define extended symmetries, which is a counterpart to that in Sect. 2.2 for standard symmetries. As stated previously, the centralizers $\mathrm{cent}_{S_n}(\varrho_j)$ can be computed for each column using Fact 2.11, and thus the problem reduces to obtaining a suitable candidate for each κ_i, which once again can be done by an application of Fact 2.11. The algorithm is as follows:

Algorithm 2. Assuming that ϱ is a primitive, bijective, aperiodic substitution, the following algorithm computes the set K of permutations that induce reversors, which determines $\mathcal{R}(\mathbb{X}_\varrho)$.

- **Input:** ϱ is a length-L bijective substitution, represented either as a function or a set of columns.
- **Output:** A (finite) set of permutations K, either empty or a coset of the group H computed by the previous algorithm, so that $\mathcal{R}(\mathbb{X}_\varrho)/\langle\sigma\rangle \simeq H \cup K$ (i.e., $\mathcal{R}(\mathbb{X}_\varrho) \simeq \mathbb{Z} \rtimes_\varphi (H \cup K)$, with $\varphi(g,n) = n$ if $g \in H$, and $-n$ if $g \in K$).

(1) Let N be the least positive integer which ensures that two opposite columns of ϱ^N are the identity map. This can be computed as:

$$N = \min\left\{\mathrm{lcm}\left(\mathrm{ord}(\varrho_i), \mathrm{ord}(\varrho_{L-(i+1)})\right) : 0 \le i \le N/2\right\}.$$

(2) For each $0 \le i \le N/2$, compute κ_i via the following subroutine:

(2.i) If ϱ_i and $\varrho_{L-(i+1)}$ are non-conjugate (i.e., their cycle decomposition has a different number of cycles of some length), stop the algorithm, as reversors do not exist (see Theorem 3.5).

(2.ii) Sort the cycles from the disjoint cycle decomposition of ϱ_i by increasing order of length. Using this as a basis, by appropriately sorting the elements of each cycle in this decomposition, define a total order relation $<$ on $\mathcal{A}$, given by, say, $a_1 < \ldots < a_n$, such that all of the elements of a given cycle come before the elements of the following cycle, in the sorting by left. Do the same for $\varrho_{L-(i+1)}$, defining a corresponding total order $<'$ given by $b_1 <' \ldots <' b_n$. This ensures that there are cycle decompositions of both permutations such that the corresponding cycles, ordered from left to right, have the same length, as follows:

$$\varrho_i = (a_1 \ \ldots \ a_j)(a_{j+1} \ \ldots \ a_{j'}) \cdots (a_{j''+1} \ \ldots \ a_n),$$
$$\varrho_{L-(j+1)} = (b_1 \ \ldots \ b_j)(b_{j+1} \ \ldots \ b_{j'}) \cdots (b_{j''+1} \ \ldots \ b_n),$$

with $1 \leq j \leq j' \leq \ldots \leq j'' \leq n$.

(2.iii) Define:

$$\kappa_i = \begin{pmatrix} a_1 & a_2 & \cdots & a_n \\ b_1 & b_2 & \cdots & b_n \end{pmatrix}, \qquad \kappa_{L-(i+1)} = \kappa_i^{-1}.$$

(3) Compute each centralizer $H^{(i)} = \mathrm{cent}_{S_n}(\varrho_i)$, using the same procedure as in the computation of $\mathcal{S}(\mathbb{X}_\varrho)$.

(4) Return $K = \bigcap_{i=1}^N H^{(i)}\kappa_i$. Any element of K induces a reversor; if K is empty, reversors do not exist.

Any programming environment with suitable data structures (e.g. computer algebra systems such as `Sagemath`® or `Mathematica`®) is amenable to the implementation of this algorithm, providing effective procedures to entirely characterize the groups $\mathcal{S}(\mathbb{X}_\varrho)$ and $\mathcal{R}(\mathbb{X}_\varrho)$ from a suitable description of the substitution ϱ, e.g. using a dictionary.

Example 3.7 Going back to Example 2.12, we may apply the previous algorithm to determine whether reversors for this substitution do exist. Following the steps of Algorithm 2, we obtain:

(1) For the algorithm to work properly, we need two columns in opposite positions to be identity columns. Since every element in the quaternion group Q_8 has order 4, we may just take $N = 4$ (and indeed, inspection shows that this is the smallest value of N that satisfies this property).

(2) It is not hard to see that the columns of ϱ^4 are, in order, R_{i^4}, $R_{i^3 j}$, $R_{i^3 k}$, $R_{i^2 ji}, \ldots,$ $R_{k^2 jk}$, $R_{k^3 i}$, $R_{k^3 j}$, R_{k^4}, and thus, due to the nature of the elements of Q_8 (namely, that the mapping that sends i and j to any two of the three elements $\{i, j, k\}$ is a group automorphism), opposite columns are conjugate. We need to find mappings κ_r such that the rth column from left to right is conjugate to the corresponding column from right to left under k. For example, the second and penultimate column are given by

$$R_{i^3 j} = R_{\bar{k}} = (e\,\bar{k}\,\bar{e}\,k)(i\,j\,\bar{\imath}\,\bar{\jmath}), \qquad R_{k^3 j} = R_i = (e\,i\,\bar{e}\,\bar{\imath})(j\,\bar{k}\,\bar{\jmath}\,k).$$

Using Fact 2.11, we see that if κ_1 is a permutation that maps $R_{i^3 j}$ to $R_{k^3 j}$ via conjugation, choosing the images of one element of the first cycle and one of the second is enough to determine the whole permutation. If $\kappa_1(e) = k$ and $\kappa_1(i) = e$, then it must map the following elements of each cycle of $R_{i^3 j}$ to the following elements of the corresponding cycle in $R_{k^3 j}$, and thus we obtain

$$\kappa_1 = \begin{pmatrix} e & i & j & k & \bar{e} & \bar{\imath} & \bar{\jmath} & \bar{k} \\ \bar{\jmath} & i & \bar{e} & \bar{k} & j & \bar{\imath} & e & k \end{pmatrix} = (e\,\bar{\jmath})(j\,\bar{e})(\bar{k}\,k).$$

Thus, any element of the coset $\mathrm{cent}_{S_8}(R_{i^3j})\kappa_1$ in S_8 maps the second column to the penultimate one by conjugation. Note that the corresponding step of Algorithm 1 above actually returns a different permutation, $\kappa_1' = (\bar{k}\ i\ j)(k\ \bar{\imath}\ \bar{\jmath})$, but direct computation shows that κ_1 and κ_1' belong to the same coset of $\mathrm{cent}_{S_8}(R_{i^3j})$ and thus the algorithm proceeds in the same way for either; we choose κ_1 instead of κ_1' for mere convenience. After this, we repeat the same procedure for the remaining 40 pairs of columns (including the center, which is paired with itself) and compute the intersection of the obtained cosets.

(3) We note that the computed permutation κ_1 appears in every coset $\mathrm{cent}_{S_8}((\varrho^4)_r)\kappa_r$, and thus the intersection of all cosets involved equals a right coset of the left Cayley embedding of Q_8 in S_8, which must equal $K = L(Q_8)\kappa_1$. It can be verified from computation that the union $L(Q_8) \cup K$ of this embedding and the corresponding coset is also a subgroup of S_8.

(4) Thus, every element of $\mathcal{R}(\mathbb{X}_\varrho)$ is associated with a letter swap from the subgroup $G = L(Q_8) \cup K$ of S_8, with reversors corresponding to elements of $K = G \setminus Q_8$. Note that this group has order 16. Besides, $\{R_e, \kappa_1\}$ is an order 2 subgroup of G with trivial intersection with Q_8, which is normal in G due to being of index 2; thus, this group has a natural semidirect product structure as $G \simeq Q_8 \rtimes C_2$. Computation aided with computer algebra software shows that this group G has fifteen subgroups and seven different conjugacy classes. The only group of order 16 with both properties is the *semidihedral group*, SD_{16}. Thus, we obtain a complete description of $\mathcal{R}(\mathbb{X})$ as the semidirect product $\mathbb{Z} \rtimes SD_{16} \simeq (\mathbb{Z} \times Q_8) \rtimes C_2$.

3.2 Higher-Dimensional Subshifts

Now, we turn our attention to the situation in higher dimensions. The *extended symmetry group* of a $\mathbb{Z}^d$-shift is defined as $\mathcal{R}(\mathbb{X}) = \mathrm{norm}_{\mathrm{Aut}(\mathbb{X})}(\mathcal{G})$, where now $\mathcal{G} = \langle \sigma_{e_1}, \ldots, \sigma_{e_d} \rangle \simeq \mathbb{Z}^d$; see [3,6,10]. In this more general context, an *extended symmetry* is an element $f \in \mathcal{R}(\mathbb{X}) \setminus \mathcal{S}(\mathbb{X})$.

Similar to standard symmetries, there is a direct generalization of the characterization of extended symmetries from Proposition 3.2 and the subsequent theorem to the higher-dimensional setting, which is given by the following.

Proposition 3.8 *Let ϱ be an aperiodic, primitive, bijective, block substitution in $\mathbb{Z}^d$. Then any extended symmetry $f \in \mathcal{R}(\mathbb{X}_\varrho) \setminus \mathcal{S}(\mathbb{X}_\varrho)$ must be (up to a shift) a composition of a permutation and a rearrangement function f_A given by $f_A(x)_{\boldsymbol{n}} = x_{A\boldsymbol{n}}$, with $A \in \mathrm{GL}(d, \mathbb{Z}) \setminus \{\mathbb{I}\}$, where $\mathbb{I}$ is the identity matrix.*

For shifts generated by bijective rectangular substitutions one has the following restriction on the linear component A of an extended symmetry f.

Theorem 3.9 [10, Thm. 18] *Let ϱ an aperiodic, primitive, bijective rectangular substitution in $\mathbb{Z}^d$. One then has*

$$\mathcal{R}(\mathbb{X}_\varrho)/\mathcal{S}(\mathbb{X}_\varrho) \simeq P \leq W_d,$$

where $W_d \simeq C_2^d \rtimes S_d$ is the d-dimensional hyperoctahedral group, which represents the symmetries of the d-dimensional cube.

Using Theorem 3.9, one can show that all extended symmetries of such subshifts are of finite order. The proof of the following result is patterned from [5, Prop. 2], which deals with the order of reversors of an automorphism h of a general dynamical system with $\mathrm{ord}(h) = \infty$; compare [23]. The crucial component here is the finiteness of W_d, which implies that all of its elements are of finite order. We note here that there exist subshifts of number-theoretic origin where $\mathcal{R}(\mathbb{X})/\mathcal{S}(\mathbb{X}) = \mathrm{GL}(d, \mathbb{Z})$, and hence for which extended symmetries of infinite order exist; see [3].

Proposition 3.10 *Let $\mathbb{X}_\varrho$ be the same as above with symmetry group $\mathcal{S}(\mathbb{X}_\varrho) = \mathbb{Z}^d \times H$. Let $f \in \mathcal{R}(\mathbb{X}_\varrho) \backslash \mathcal{S}(\mathbb{X}_\varrho)$ be an extended symmetry, whose associated matrix is $A \in W_d$. Then* $\mathrm{ord}(f)$ *divides* $\mathrm{ord}(A) \cdot |H|$. *Moreover,* $\mathrm{ord}(f) \leq 2|H| \cdot \max\{\mathrm{ord}(\tau) : \tau \in S_d\}$.

Proof From Proposition 3.8, $f \circ \sigma_{\boldsymbol{m}} \circ f^{-1} = \sigma_{A\boldsymbol{m}}$ holds for all $\boldsymbol{m} \in \mathbb{Z}^d$, which yields

$$f^{\ell} \circ \sigma_{\boldsymbol{m}} \circ f^{-\ell} = \sigma_{A^{\ell}\boldsymbol{m}} \tag{7}$$

$$f \circ \sigma_{n\boldsymbol{m}} \circ f^{-1} = \sigma_{nA\boldsymbol{m}} \tag{8}$$

for all $\ell, n \in \mathbb{N}$. Choosing $\ell = \mathrm{ord}(A)$, (7) gives $f^{\mathrm{ord}(A)} \in \mathcal{S}(\mathbb{X}_\varrho)$. From Theorem 2.8, $f^{\mathrm{ord}(A)} = \sigma_{\boldsymbol{p}} \circ \pi$, for some $\boldsymbol{p} \in \mathbb{Z}^d$ and letter-exchange map π. From the direct product structure of the symmetry group, one has $\sigma_{\boldsymbol{p}} \circ \pi = \pi \circ \sigma_{\boldsymbol{p}}$, which implies $f^{\mathrm{ord}(A) \cdot |H|} = \sigma_{|H|\boldsymbol{p}} \circ \pi^{|H|} = \sigma_{|H|\boldsymbol{p}}$. Using the two equations above, one gets $f^{\mathrm{ord}(A) \cdot |H|} = \sigma_{|H|A^{\ell}(\boldsymbol{p})}$ for all $\ell \in \mathbb{N}$. Since f is an extended symmetry, $A \neq \mathbb{I}$. Next we show that $\boldsymbol{p}$ cannot be an eigenvector of A.

Suppose $A\boldsymbol{p} = \boldsymbol{p}$ with $\boldsymbol{p} \neq \boldsymbol{0}$. Note that $f^{-\mathrm{ord}(A)|H|} = \sigma_{-|H|\boldsymbol{p}}$. From (7) and (8), one also has $f^{-1} \circ \sigma_{|H|A^{-1}\boldsymbol{p}} \circ f = \sigma_{-|H|\boldsymbol{p}}$, which implies $A^{-1}\boldsymbol{p} = -\boldsymbol{p}$, contradicting the assumption on $\boldsymbol{p}$. Since $\mathrm{ord}(\sigma_{\boldsymbol{p}}) = \infty$, this forces $\boldsymbol{p} = \boldsymbol{0}$ and hence $f^{\mathrm{ord}(A) \cdot |H|} = \mathrm{id}$ from which the first claim is immediate. The upper bound for the order follows from the upper bound for the order of the elements of the hyperoctahedral group W_d; see [2]. □

Due to the fact that $\mathcal{R}(\mathbb{X}_\varrho)$ is (possibly) a larger extension of $\mathcal{S}(\mathbb{X}_\varrho)$ (that is, the corresponding quotient can have up to $2^d d! - 1$ non-trivial elements instead of just one), we would end up with a much larger number of equations of the form of (2), one for each element of the hyperoctahedral group W_d except the identity. This leads us to another problem of different nature: if the rectangle R, which is the support of the level-1 supertiles of ϱ, is not a cube in $\mathbb{Z}^d$, some symmetries from W_d may not be compatible with R, i.e., they may map R to a different rectangle that is not a translation of R, so the corresponding equation does not have a proper meaning (as it may compare an existing column with a non-existent one).

This could be taken as a suggestion that such symmetries cannot actually happen, imposing further limitations on the quotient $\mathcal{R}(\mathbb{X}_\varrho)/\mathcal{S}(\mathbb{X}_\varrho)$. Interestingly, this is not actually the case. For instance, consider the two-dimensional rectangular substitution from Fig. 2. As the support for this substitution is a 4×2 rectangle, we could guess that this substitution is incompatible with rotational symmetries or reflections along

Fig. 2 A non-square substitution that generates the two-dimensional Thue–Morse subshift

a diagonal axis, which would produce a 2×4 rectangle instead. However, further examination shows that the subshift generated by this substitution is actually the same as the subshift of the two-dimensional Thue–Morse substitution as seen in e.g. [10], which is compatible with every symmetry from $W_2 = D_4$. Thus, only geometrical considerations are not enough to exclude candidates for extended symmetries.

Fortunately, there is a subcase of particular interest in which this geometrical intuition is actually correct, which involves an arithmetic restriction on the side lengths of the support rectangle R. It turns out that coprimality of the side lengths is a sufficient condition (although it can be weakened even further) to rule out such symmetries, e.g. there are no extended symmetries compatible with rotations when R is a, say, 2×5 rectangle. The following result makes this observation precise, providing a sufficient criterion to rule out the existence of certain extended symmetries.

Theorem 3.11 *Let $\varrho \colon \mathcal{A} \to \mathcal{A}^R$ be a bijective rectangular substitution with faithful associated shift action. Suppose that $R = [\mathbf{0}, \boldsymbol{L} - \mathbf{1}]$ with $\boldsymbol{L} = (L_1, \ldots, L_d)$ (that is, R is a d-dimensional rectangle with side lengths $L_1, L_2, \ldots, L_d$) and that for some indices i, j there is a prime p such that $p \mid L_j$ but $p \nmid L_i$, i.e., L_i and L_j have different sets of prime factors. Let $A \in W_d \leq \mathrm{GL}(d, \mathbb{Z})$ and suppose that A is the underlying matrix associated to an extended symmetry $f \in \mathcal{R}(\mathbb{X}_\varrho)$. Then $A_{ij} = A_{ji} = 0$.*

The underlying idea is that, if $A \in W_d$ induces a valid extended symmetry for some substitution ϱ with support U, we can find another substitution η with support $A \cdot U$ (up to an appropriate translation) such that $\mathbb{X}_\varrho = \mathbb{X}_\eta$, and then we use the known factor map from an aperiodic substitutive subshift onto an associated odometer to rule out certain matrices A. Similar exclusion results have been studied by Cortez and Durand [12].

Proof Let $\varphi \colon \mathbb{X}_\varrho \twoheadrightarrow \mathbb{Z}_{L_1} \times \cdots \times \mathbb{Z}_{L_d} = \mathbb{Z}_{\boldsymbol{L}}$ be the standard factor map from the substitutive subshift to the corresponding product of odometers. It is known [6, Thm. 5] that, for any extended symmetry $f \colon \mathbb{X}_\varrho \to \mathbb{X}_\varrho$ with associated matrix A, there exists $\boldsymbol{k}_f = (k_1, \ldots, k_d) \in \mathbb{Z}_{\boldsymbol{L}}$ and a group automorphism $\alpha_f \colon \mathbb{Z}_{\boldsymbol{L}} \to \mathbb{Z}_{\boldsymbol{L}}$ satisfying the following equation:

$$\varphi(f(x)) = \boldsymbol{k}_f + \alpha_f(\varphi(x)), \tag{9}$$

where α_f is the unique extension of the map $\boldsymbol{n} \mapsto A\boldsymbol{n}$, defined in the dense subset $\mathbb{Z}^d$, to $\mathbb{Z}_{\boldsymbol{L}}$. In particular, for any $\boldsymbol{n} \in \mathbb{Z}^d$, if $f = \sigma_{\boldsymbol{n}}$ is a shift map, then $\boldsymbol{k}_{\sigma_{\boldsymbol{n}}} = \boldsymbol{n}$ and $\alpha_{\sigma_{\boldsymbol{n}}} = \mathrm{id}_{\mathbb{Z}_{\boldsymbol{L}}}$.

Now, consider the sequence $\boldsymbol{h}_m = L_i^m \boldsymbol{e}_i$, and suppose $A_{ji} = \pm 1$. Equivalently, $A\boldsymbol{e}_i = \pm \boldsymbol{e}_j$, since A is a signed permutation matrix. Without loss of generality, we may assume the sign to be $+$. One has $L_i^m \xrightarrow{m\to\infty} 0$ in the L_i-adic topology, and thus $\varphi(\sigma_{\boldsymbol{h}_m}(x)) = \boldsymbol{h}_m + \varphi(x) \xrightarrow{m\to\infty} \varphi(x)$, as it does so componentwise. By compactness, we may take a subsequence $\boldsymbol{h}_{\beta(m)}$ such that $\sigma_{\boldsymbol{h}_{\beta(m)}}(x)$ converges to some x^*; then, as the factor map φ is continuous, we have $\varphi(x^*) = \varphi(x)$.

Equation (9) and this last equality imply that $\varphi(f(x)) = \varphi(f(x^*))$ as well. Writing x^* as a limit, we obtain from continuity that

$$\begin{aligned}\varphi(x^*) &= \lim_{m\to\infty} \varphi(f(\sigma_{\boldsymbol{h}_{\beta(m)}}(x))) = \lim_{m\to\infty} \varphi(\sigma_{A\boldsymbol{h}_{\beta(m)}}(f(x))) \\ &= \varphi(x) + \lim_{m\to\infty} A\boldsymbol{h}_{\beta(m)} = \varphi(x) + \lim_{m\to\infty} L_i^{\beta(m)} A\boldsymbol{e}_i \\ \implies \quad & \lim_{m\to\infty} L_i^{\beta(m)} \boldsymbol{e}_j = \varphi(x^*) - \varphi(x) = \mathbf{0}.\end{aligned}$$

The last equality implies that, in the topology of $\mathbb{Z}_{L_j}$, the sequence $L_i^{\beta(m)}$ converges to 0. However, since there is a prime p that divides L_j but not L_i, due to transitivity we must have $L_j \nmid L_i^n$ for all n, as otherwise $p \mid L_i^n$ and thus $p \mid L_i$. Thus, in base L_j, the last digit of $L_i^{\beta(m)}$ is never zero, and thus $L_i^{\beta(m)}$ remains at fixed distance 1 from $\mathbf{0}$ (in the L_j-adic metric), contradicting this convergence. Thus, A_{ji} cannot be 1 and must necessarily equal 0. For A_{ij}, the same reasoning applies to f^{-1}, which is associated to A^{-1}. Since A is a signed permutation matrix, $A_{ij} = \pm 1$ would imply $(A^{-1})_{ji} = \pm 1$, again a contradiction. □

We now proceed to the generalization of Theorem 3.5 in higher dimensions. As before, for a block substitution ϱ, we have $R = \prod_{i=1}^d [0, L_i - 1]$, with $L_i \geq 2$ and the expansive map $Q = \mathrm{diag}(L_1, L_2, \ldots, L_d)$. Let $A \in W_d \leq \mathrm{GL}(d, \mathbb{Z})$ be a signed permutation matrix. First, we assume that the location of a tile in any supertile is given by the location of its center. Define the affine map $A^{(1)} \colon R \to R$ via $A^{(1)}(\boldsymbol{i}) = A(\boldsymbol{i} - \boldsymbol{x}_1) + |A|\boldsymbol{x}_1$ where $\boldsymbol{i} \in R$ and $\boldsymbol{x}_1 = Q\boldsymbol{v} - \boldsymbol{v}$ with $\boldsymbol{v} = (1/2)(1, 1, \ldots, 1)^T$. Here, $(|A|)_{ij} = |A_{ij}|$. The vector $|A|\boldsymbol{x}_1$ is the translation needed to shift the center of the supertile to the origin, which we will need before applying the map A and shifting it back again. We extend $A^{(1)}$ to any level-k supertile by defining the map $A^{(k)} \colon R^{(k)} \to R^{(k)}$ given by

$$A^{(k)}(\boldsymbol{i}) = A(\boldsymbol{i} - \boldsymbol{x}_k) + |A|\boldsymbol{x}_k, \tag{10}$$

with $\boldsymbol{i} \in R^{(k)}$ and $\boldsymbol{x}_k = Q^k\boldsymbol{v} - \boldsymbol{v}$. Here $R^{(k)} := \prod_{i=1}^d [0, L_i^k - 1]$ is the set of locations of tiles in a level-k supertile.

Example 3.12 Let ϱ be a two-dimensional block substitution with

$$Q = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

and A be the counterclockwise rotation by 90°, with corresponding matrix

$$A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

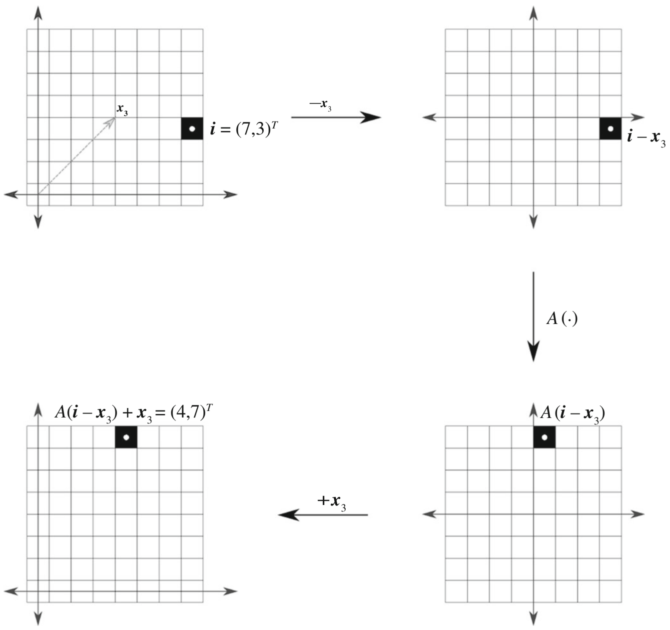


Fig. 3 The transformation of a marked level-3 location set $R^{(3)}$ under the map $A^{(3)}$

Consider the level-3 supertile and let $\boldsymbol{i} = (7,3)^T \in R^{(3)}$, with Q-adic expansion $\boldsymbol{i} \mathrel{\widehat{=}} \boldsymbol{i}_2\boldsymbol{i}_1\boldsymbol{i}_0$. Here one has $\boldsymbol{i}_0 = \boldsymbol{i}_1 = \boldsymbol{e}_1 + \boldsymbol{e}_2$ and $\boldsymbol{i}_2 = \boldsymbol{e}_1$. One then gets $A^{(3)}(\boldsymbol{i}) = (4,7)^T$; see Fig. 3. One can check that $\sum_{j=0}^{2} Q^j(A^{(1)}(\boldsymbol{i}_j)) = A^{(3)}(\boldsymbol{i})$.

The following result is the analog of Theorem 3.5 in $\mathbb{Z}^d$. Most parts of the proof mimics those of the proof of Theorem 3.5, where one replaces the mirroring operation m with a more general map $A \in W_d$.

Theorem 3.13 *Let ϱ be an aperiodic, primitive, bijective block substitution $\varrho\colon \mathcal{A} \to \mathcal{A}^R$. Let W_d be the d-dimensional hyperoctahedral group and let $A \in W_d$. Suppose there exists $\boldsymbol{\ell} \in R$ such that $\varrho_{\boldsymbol{\ell}'} = \mathrm{id}$ for all $\boldsymbol{\ell}' \in \mathrm{Orb}_A(\boldsymbol{\ell})$. Assume further that $[A, Q] = 0$ and $|A|\boldsymbol{x}_1 = \boldsymbol{x}_1$. Then π, together with A, gives rise to an extended symmetry $f \in \mathcal{R}(\mathbb{X}_\varrho)$ if and only if*

$$\pi^{-1} \circ \varrho_{\boldsymbol{i}} \circ \pi = \varrho_{A^{(1)}(\boldsymbol{i})} \tag{11}$$

for all $\boldsymbol{i} \in R$.

Proof In higher dimensions, the form of an extended symmetry is given in Proposition 3.8. From this and from the assumptions above, one gets an analogous system of equations as in those coming from (3) in the proof of Proposition 3.4 which one can use directly to show the necessity direction.

To prove sufficiency, we show that if (11) is satisfied for all $\boldsymbol{i} \in R$, then it also holds for all positions in any level-k supertile. Let $\boldsymbol{i} \in R^{(k)}$, which admits the unique Q-adic expansion given by $\boldsymbol{i} \,\widehat{=}\, \boldsymbol{i}_{k-1}\boldsymbol{i}_{k-2}\ldots\boldsymbol{i}_1\boldsymbol{i}_0$, i.e., $\boldsymbol{i} = \sum_{j=0}^{k-1} Q^j(\boldsymbol{i}_j)$. We now show that the Q-adic expansion of $A^{(k)}(\boldsymbol{i})$ is given by $A^{(k)}(\boldsymbol{i}) \,\widehat{=}\, A^{(1)}(\boldsymbol{i}_{k-1})A^{(1)}(\boldsymbol{i}_{k-2})\ldots A^{(1)}(\boldsymbol{i}_0)$. Plugging in the expansion of $\boldsymbol{i}$ into (10), one gets $A^{(k)}(\boldsymbol{i}) = \sum_{j=0}^{k-1} AQ^j(\boldsymbol{i}_j) - A\boldsymbol{x}_k + \boldsymbol{x}_k$. On the other hand, one also has

$$
\begin{aligned}
\sum_{j=0}^{k-1} Q^j(A^{(1)}(\boldsymbol{i}_j)) &= \sum_{j=0}^{k-1} Q^j\big(A(\boldsymbol{i} - Q\boldsymbol{v} + \boldsymbol{v}) + Q\boldsymbol{v} - \boldsymbol{v}\big) \\
&= \sum_{j=0}^{k-1} Q^j A(\boldsymbol{i}_j) + \sum_{j=0}^{k-1}(-AQ^{j+1}\boldsymbol{v} + AQ^j\boldsymbol{v}) + \sum_{j=0}^{k-1}(Q^j\boldsymbol{v} - Q^j\boldsymbol{v}) \\
&= \sum_{j=0}^{k-1} AQ^j(\boldsymbol{i}_j) \underbrace{- AQ^k\boldsymbol{v} + A\boldsymbol{v}}_{-A\boldsymbol{x}_k} + \underbrace{Q^k\boldsymbol{v} - \boldsymbol{v}}_{\boldsymbol{x}_k} = A^{(k)}(\boldsymbol{i}),
\end{aligned}
$$

where the penultimate equality follows from $[A, Q] = 0$ and the evaluation of the two telescoping sums. As in Theorem 3.5, one then obtains

$$
\pi^{-1} \circ \varrho_{\boldsymbol{i}} \circ \pi = \pi^{-1} \circ \varrho_{\boldsymbol{i}_{k-1}} \circ \varrho_{\boldsymbol{i}_{k-2}} \circ \cdots \circ \varrho_{\boldsymbol{i}_0} \circ \pi = \varrho_{A^{(k)}(\boldsymbol{i})},
$$

whenever $\boldsymbol{i} \,\widehat{=}\, \boldsymbol{i}_{k-1}\boldsymbol{i}_{k-2}\ldots\boldsymbol{i}_0$ and $\pi^{-1} \circ \varrho_{\boldsymbol{i}_s} \circ \pi = \varrho_{A^{(1)}(\boldsymbol{i}_s)}$ for all $\boldsymbol{i}_s \in R$, which finishes the proof. $\square$

Remark 3.14 The conditions $[A, Q] = 0$ and $|A|\boldsymbol{x}_1 = \boldsymbol{x}_1$ in Theorem 3.13 are automatically satisfied if ϱ is a cubic substitution, i.e., $L_i = L$ for all $1 \leq i \leq d$, which means one can use (11) to check whether a given letter-exchange map works for any $A \in W_d$. For general ϱ, these relations are only satisfied for certain $A \in W_d$, e.g. reflections along coordinate axes, which means one needs a different tool to ascertain whether it is possible for other rigid motions to generate extended symmetries. For example, one can use Theorem 3.11 to exclude some symmetries.

Before we proceed, we need a higher-dimensional generalization of Proposition 2.5 regarding aperiodicity. For this, we use the following result, which is formulated in terms of Delone sets. Here, $\mathbb{S}^{d-1}$ is the unit sphere in $\mathbb{R}^d$.

Theorem 3.15 [4, Thm. 5.1] *Let $\mathbb{X}(\varLambda)$ be the continuous hull of a repetitive Delone set $\varLambda \subset \mathbb{R}^d$. Let $\{\boldsymbol{b}_i \in \mathbb{S}^{d-1} : 1 \leq i \leq d\}$ be a basis of $\mathbb{R}^d$ such that for each i, there are two distinct elements of $\mathbb{X}(\varLambda)$ which agree on the half-space $\{\boldsymbol{x} : \langle \boldsymbol{b}_i | \boldsymbol{x}\rangle > \alpha_i\}$ for some $\alpha_i \in \mathbb{R}^d$. Then one has that $\mathbb{X}(\varLambda)$ is aperiodic.*

The proof of the previous theorem relies on the generalization of the notion of proximality for tilings and Delone sets in $\mathbb{R}^d$, which is proximality along $\boldsymbol{s} \in \mathbb{S}^{d-1}$; see [4, Sect. 5.5] for further details. Note that from a $\mathbb{Z}^d$-tiling generated by a rectangular substitution, one can derive a (colored) Delone set $\varLambda$ by choosing a consistent control point for each cube (usually one of the corners or the center). Primitivity guarantees that $\varLambda$ is repetitive and the notion of proximality extends trivially to colored Delone sets using the same metric. The two subshifts $\mathbb{X}(\varLambda)$ and $\mathbb{X}_\varrho$ are then mutually locally

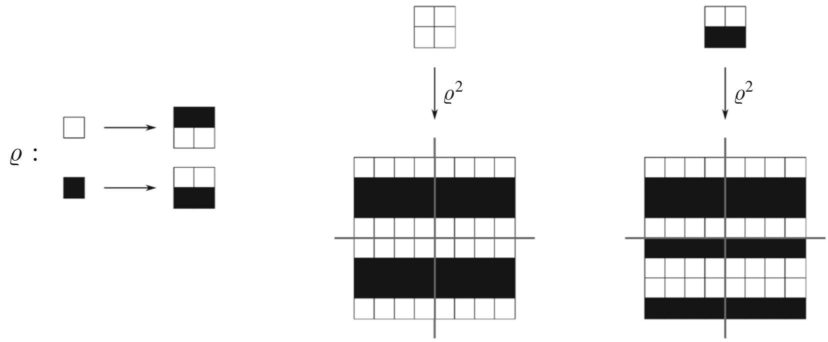


Fig. 4 The image of two distinct blocks under ϱ coincide in the upper half-plane and are distinct in the lower half-plane. In the limit, these legal seeds generate two fixed points which are neither left nor right asymptotic with respect to $\sigma_{\boldsymbol{e}_1}$

derivable, and the aperiodicity of one implies that of the other. We then have a sufficient criterion for the aperiodicity of $\mathbb{X}_\varrho$ in higher dimensions.

Proposition 3.16 *Let $\varrho\colon \mathcal{A} \to \mathcal{A}^R$ be a d-dimensional rectangular substitution which is bijective and primitive. If there exist two legal blocks $u, v \in \mathcal{L}$ of side-length 2 in each direction such that u and v disagrees at exactly one position and coincides at all other positions, then the subshift $\mathbb{X}_\varrho$ is aperiodic.*

Proof The proof proceeds in analogy to Proposition 2.5. Here we choose the appropriate power to be

$$k = \operatorname{lcm}\left\{ |\varrho_{\boldsymbol{r}}| : \boldsymbol{r} = \sum_{i=1}^{d} r_i \boldsymbol{e}_i,\ r_i \in \{0, L_i - 1\} \right\}.$$

If we then place u and v at the origin, the resulting fixed points $x = \varrho^\infty(u)$ and $x' = \varrho^\infty(v)$ which cover $\mathbb{Z}^d$ will coincide at every sector except at the one where $u_{\boldsymbol{j}} \neq v_{\boldsymbol{j}}$. One can then choose $\boldsymbol{b}_i = \boldsymbol{e}_i$ and $\alpha_i = 0$ in Theorem 3.15, and for each i, x, and x' to be the two elements which agree on a half-space, which guarantees the aperiodicity of $\mathbb{X}_\varrho$. More concretely, x and x' are asymptotic, and hence proximal, along $\boldsymbol{e}_i$ for all $1 \leq i \leq d$. $\square$

Remark 3.17 Obviously, one can have a lattice of periods of rank less than d in higher dimensions. An example would be when $\varrho = \varrho_1 \times \varrho_2$, where ϱ_1 is the trivial substitution $a \mapsto aa$, $b \mapsto bb$, and ϱ_2 is Thue–Morse. Although ϱ_1 is itself not primitive, the product ϱ is and admits the legal blocks given in Fig. 4, which generate fixed points that are $\mathbb{Z}\boldsymbol{e}_1$-periodic. If one requires that the shift component in $\mathcal{S}(\mathbb{X}_\varrho)$ is $\mathbb{Z}^d$, one needs all elements of $\mathbb{X}_\varrho$ to be aperiodic in all cardinal directions, hence the stronger criterion in Proposition 3.16.

The next result is the analog of Theorem 2.13 for extended symmetries, which holds in any dimension.

Theorem 3.18 *Given a finite group H and a subgroup P of the d-dimensional hyperoctahedral group W_d, there is an aperiodic, primitive, bijective d-dimensional substitution ϱ whose subshift satisfies*

$$\mathcal{S}(\mathbb{X}_\varrho) \simeq \mathbb{Z}^d \times H, \qquad \mathcal{R}(\mathbb{X}_\varrho) \simeq (\mathbb{Z}^d \rtimes P) \times H.$$

Proof We start by taking a cursory look at the proof of [17, Thm. 3.6]. For a given finite group H, we choose a generating set $S = \{s_1, \ldots, s_r\}$, and build a substitution whose columns correspond to the left multiplication maps $L_{s_j}(h) = s_j \cdot h$, seen as permutations of the alphabet $\mathcal{A} = H$, plus an identity column if necessary so that $G^{(N)} = G^{(1)}$ for all N. These permutations generate the left Cayley embedding of H in the symmetric group on $|H|$ elements, whose corresponding centralizer, which induces all of the letter exchanges in $\mathcal{S}(\mathbb{X}_\varrho)$, is the right Cayley embedding of H generated by the maps $R_{s_j}(h) = h \cdot s_j$. By construction, these columns generate a transitive subgroup, which ensures primitivity by Proposition 2.3.

In what follows, we shall assume first that the group H is non-trivial, as the case in which H is trivial requires a slightly different construction. We also assume that the rectangular substitution we will construct engenders an aperiodic subshift, so that the group generated by the shifts is isomorphic to $\mathbb{Z}^d$. We delay the proof of this until later on, to avoid cluttering our construction with extraneous details.

Since $\mathcal{S}(\mathbb{X}_\varrho)$ depends only on the columns of the underlying substitution and not their relative position, we shall construct a d-dimensional rectangular substitution ϱ with cubic support whose columns correspond to copies of the aforementioned L_{s_j}, placed in adequate positions along the cube. We start with a cube $R = [0, 2|S| + 2d + 1]^d$ of side length $2|S| + 2d + 2$, where the additional layer corresponding to the term 2 will be used below to ensure aperiodicity. This cube is comprised of $N = |S| + d + 1$ "shells" or "layers", which are the boundaries of the inner cubes $[j, 2|S| + 2d + 2 - j]^d$; we shall denote each of them by Λ_j, where j can vary from 0 to $N - 1$.

Fill the ith inner shell Λ_{N-i} with copies of the column L_{s_i}, for all $1 \le i \le r$. This ensures that, as long as every other column is a copy of L_{s_j} for some j or an identity column, the symmetry group $\mathcal{S}(\mathbb{X}_\varrho)$ of the corresponding subshift will be isomorphic to H, because in our construction the 2^d corners of the point will always be identity columns.

Now, note that N is chosen large enough so that the point $\boldsymbol{p} = (0, 1, \ldots, d-1)$ lies in the outer $N - r \ge d$ shells and, moreover, the cube $[0, d-1]^d$ is contained in these outer shells as well. Thus, any permutation of the coordinates maps the cube $[0, d-1]^d$ to itself and, in particular, two different permutations map this point to two different points in this cube, that is, the orbit of $\boldsymbol{p}$ has $d!$ different points. Combining this with the fact that the mirroring maps send this cube to one of 2^d disjoint cubes (translations of $[0, d-1]^d$) in the corners of the larger cube $[0, N-1]^d$, it can be seen that W_d acts freely on the orbit of the point $\boldsymbol{p}$, that is, there is a bijection between the hyperoctahedral group W_d and the set $\mathrm{Orb}(\boldsymbol{p})$.

Next, choose a fixed $s_j \in S$ that is not the identity element of H, so that L_{s_j} is not an identity column. As P is a subgroup of W_d, it is bijectively mapped to the set $P \cdot \boldsymbol{p} = \{h \cdot \boldsymbol{p} : h \in P\}$. Place a copy of L_{s_j} in each position from $P \cdot \boldsymbol{p}$, and an

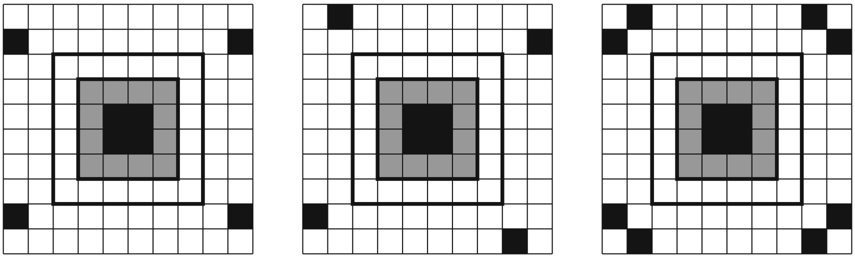


Fig. 5 Examples of substitutions obtained by the above construction, for the Klein 4-group $C_2 \times C_2$, the cyclic group C_4 and the whole $W_2 = D_4$, respectively. The thicker lines mark the layer of identity columns separating the inner cube from the outer shell

identity column in every other position from $\mathrm{Orb}(\boldsymbol{p})$. Fill every remaining position in the cube with identity columns; see Fig. 5. This ensures that the group of letter exchanges will remain isomorphic to H, and, for each matrix $A \in W_d$ associated with some element $h \in P$, the map f_A given by the relation $f_A(x)_{\boldsymbol{n}} = x_{A\boldsymbol{n}}$ will be a valid extended symmetry, as a consequence of Theorem 3.13.

Since every other extended symmetry is a product of such an f_A with some letter-exchange map that has to satisfy the conditions given by (11) in Theorem 3.13 due to our construction, and L_{s_j} cannot be conjugate to the identity column, the only other extended symmetries are compositions of the already extant f_A with elements from $\mathcal{S}(\mathbb{X}_\varrho)$, i.e., $\mathcal{R}(\mathbb{X}_\varrho)/\mathcal{S}(\mathbb{X}_\varrho)$ has the equivalence classes of each f_A as its only elements. As the set of all f_A is an isomorphic copy of P contained in $\mathcal{R}(\mathbb{X}_\varrho)$, we conclude that $\mathcal{R}(\mathbb{X}_\varrho)$ is isomorphic to the semi-direct product $\mathcal{S}(\mathbb{X}_\varrho) \rtimes P$. However, since every letter exchange from H commutes with every f_A trivially, this semi-direct product may be written as $\mathcal{R}(\mathbb{X}_\varrho) \simeq (\mathbb{Z}^d \rtimes P) \times H$, as desired.

In the case where H is trivial, we may choose an alphabet with at least three symbols (to ensure that $S_{|\mathcal{A}|}$ is non-Abelian) and repeat the construction above with a collection of columns $\varrho_0, \ldots, \varrho_{r-1}$ that generates some subgroup of $S_{|\mathcal{A}|}$ with trivial centralizer. For instance, this triviality is ensured if at least two columns generate $S_{|\mathcal{A}|}$. The rest of the proof proceeds in the same way.

To properly conclude the proof, we need to verify that the constructed substitution generates an aperiodic subshift. We focus on the case $d > 1$, as the one-dimensional case is a straightforward modification of the construction from Theorem 2.13. Since our d-dimensional cube has at least $d+1 \geq 3$ outer layers, we see that there is a $2 \times \cdots \times 2$ cube R_0 contained in the outer layers that does not overlap any of the 2^d cubes of size $d \times \cdots \times d$ on the corners nor the inner cube of size $2|S| \times \cdots \times 2|S|$. As a consequence, this cube R_0 contains only identity columns. We have a layer Λ_d consisting only of identity columns directly enveloping the inner cube $\Lambda_{d+1} \cup \cdots \cup \Lambda_{d+|S|}$. Hence, the layer immediately following Λ_d consists only of non-identity columns, which are copies of the same bijection $\pi : \mathcal{A} \to \mathcal{A}$. The 2^d corners of the hollow cube $\Lambda_d \cup \Lambda_{d+1}$ are then $2 \times \cdots \times 2$ cubes $R_1, \ldots, R_{2^d}$ having exactly one non-identity column each, with this non-identity column τ being placed in every one of the 2^d possible positions on these cubes.

Since τ is not the identity, there must exist some $a \in \mathcal{A}$ such that $\tau(a) \neq a$. The previous discussion thus implies that there is an admissible pattern P_a of size $2 \times \cdots \times 2$

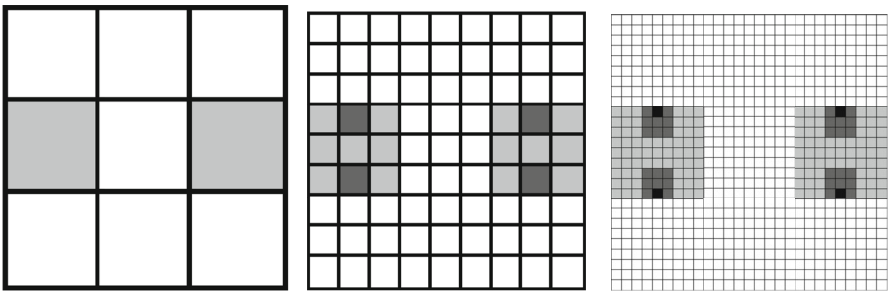
comprised only of copies of the symbol a, and $2^d + 1$ other admissible patterns $P_a^{(\boldsymbol{n})}$ that differ from P_a only in the position $\boldsymbol{n} \in [0, 1]^d$. Using the proximality criterion from Proposition 3.16, we conclude that the subshift obtained is indeed aperiodic, as desired. □

Remark 3.19 An alternative Cantor-type construction, which produces the prescribed symmetry and extended symmetry groups, involves putting the non-trivial columns on the faces of R and labelling all columns in the interior to be the identity. Let H and P be given. From Theorem 2.13, there exists a substitution on $\mathcal{A}$ with $\mathcal{S}(\mathbb{X}_\varrho) = \mathbb{Z} \times H$. Let $\varrho_0, \ldots, \varrho_{r-1}$ be the non-trivial columns of ϱ. Pick L to be large enough such that W_d acts freely on the faces of $R = [0, L-1]^d$. Choose $\boldsymbol{j}_0 \in R$ and consider the orbit of $\boldsymbol{j}_0$ under P, i.e., $\mathcal{O}_0 := P \cdot \boldsymbol{j}_0 = \{A \cdot \boldsymbol{j}_0 : A \in P\}$ where $A \cdot \boldsymbol{j} = A^{(1)}(\boldsymbol{j})$ as in (10). Label all the columns in $\mathcal{O}_0$ with ϱ_0. We then expand R via $Q = \mathrm{diag}(L, \ldots, L)$ to get the d-dimensional cube $Q(R)$ of side length L^2. Consider $\mathcal{B}_1 := Q(\mathcal{O}_0) + R$, pick $\boldsymbol{j}_1 \in \mathcal{B}_1$ and let $\mathcal{O}_1 = P \cdot \boldsymbol{j}_1$. Relabel all columns in $\mathcal{B}_1 \setminus \mathcal{O}_1$ with ϱ_0 and all columns in $\mathcal{O}_2$ with ϱ_1. One can continue this process until all needed column labels appear; see Fig. 6 for a two-dimensional example.

Note that one has $\varrho_{\boldsymbol{i}} = \varrho_{A^{(1)}(\boldsymbol{i})}$ for all $A \in P$ and $\boldsymbol{i} \in R = [0, L-1]^d$ by construction, which means $\pi = \mathrm{id}$ gives rise to an element of $\mathcal{R}(\mathbb{X}_\varrho)$ for all $A \in P$ by Theorem 3.13. No other extended symmetries can occur because all the location sets $\mathcal{B}_i$ only contain non-trivial labels and are P-invariant, whereas if $A \notin P$ induces an extended symmetry, one must have $\varrho_{\boldsymbol{\ell}} = \mathrm{id}$ for some $\boldsymbol{\ell} \in \mathcal{B}_r$.

The resulting block substitution is primitive, since reordering the columns does not affect primitivity. It is also aperiodic because one has enough identity columns, and hence one can find the legal words required in Proposition 3.16. For example, in the constructed substitution in Fig. 6, the legal seeds can be derived from the 2×2 block consisting of all identity columns (i.e., all white squares), and another one with all columns being the identity except at exactly one corner, where it is light gray. This completes the picture and one has $\mathcal{S}(\mathbb{X}_\varrho) \simeq \mathbb{Z}^d \times H$ and $\mathcal{R}(\mathbb{X}_\varrho) \simeq (\mathbb{Z}^d \rtimes P) \times H$.

We now turn our attention to examples where the letter-exchange map π that generates $f \in \mathcal{R}(\mathbb{X}_\varrho)$ is not given by the identity. In particular, in these examples, π does not commute with the letter-exchanges which correspond to the standard symmetries in



(a) $\mathcal{O}_0$ in light gray **(b)** $\mathcal{B}_1 \setminus \mathcal{O}_1$ in light gray, $\mathcal{O}_1$ in dark gray **(c)** $\mathcal{B}_2 \setminus \mathcal{O}_2$ in black

Fig. 6 An example in $\mathbb{Z}^2$ with three non-trivial columns ϱ_0 (light gray), ϱ_1 (dark gray) and ϱ_2 (black). Here, one has $H = \mathrm{cent}_{S_{|\mathcal{A}|}} \langle \varrho_0, \varrho_1, \varrho_2 \rangle$ and $P \simeq V_4$, where $V_4 \leq D_4 = W_2$ is the Klein-4 group

$\mathcal{S}(\mathbb{X}_\varrho)$. To avoid confusion, we will use letters for our substitution and the action of the hyperoctahedral group will be given by numbers, seen as permutations of the coordinates. Mirroring along a hyperplane will be denoted by m_i, where i is the respective coordinate.

Example 3.20 We explicitly give a substitution ε whose symmetry group is $\mathcal{S}(\mathbb{X}_\varepsilon) = \mathbb{Z}^d \times C_3$ and build another C_3 component in $\mathcal{R}(\mathbb{X}_\varepsilon)$, which produces reversors of order 9. With the requirement on $\mathcal{R}(\mathbb{X}_\varepsilon)/\mathcal{S}(\mathbb{X}_\varepsilon)$, the space has to be at least of dimension 3. Apart from the identity, we use the following permutations as columns:

$$\begin{aligned} \mathbf{A} &= (a\,d\,g)(b\,e\,h)(c\,f\,i), & \mathbf{B} &= (a\,b\,c)(d\,e\,f)(g\,h\,i),\\ \mathbf{E} &= (a\,g\,d)(b\,h\,e)(c\,i\,f), & \mathbf{C} &= (b\,c\,d)(e\,f\,g)(h\,i\,a),\\ & & \mathbf{D} &= (c\,d\,e)(f\,g\,h)(i\,a\,b). \end{aligned}$$

Here one has $\mathcal{S}(\mathbb{X}_\varepsilon) = \mathbb{Z}^3 \times C_3$, which is generated by $(a\,d\,g)(b\,e\,h)(c\,f\,i)$. Depending on the positioning of the columns, $\mathcal{R}(\mathbb{X}_\varepsilon)$ can either be $\mathbb{Z}^3 \rtimes C_9$, $\mathbb{Z}^3 \rtimes C_3 \times C_3$ or $\mathbb{Z}^3 \times C_3$. The group $\mathbb{Z}^3 \rtimes C_3 \times C_3$ can be realized using the construction from Theorem 3.18. On the other hand, $\mathbb{Z}^3 \times C_3$ is obtained if one orbit of maximal size is labeled with just one non-identity say $\mathbf{B}$ once, while the remaining positions in the orbit are filled with the identity.

Note that $\pi = (a\,b\,c\,d\,e\,f\,g\,h\,i)$ sends $\mathbf{B} \to \mathbf{C} \to \mathbf{D} \to \mathbf{B}$ and $\mathbf{A} \to \mathbf{A}$, $\mathbf{E} \to \mathbf{E}$. Taking the cube of $(a\,b\,c\,d\,e\,f\,g\,h\,i)$ gives $(a\,d\,g)(b\,e\,h)(c\,f\,i) \in \operatorname{cent}_{S_9}(G^{(1)})$, where $G^{(1)}$ is the group generated by the columns. This is consistent with the bounds calculated in Proposition 3.10. We will illustrate the positioning of a few elements following the construction in Theorem 3.18 with the origin being the front left lower corner; see Fig. 7. We look at a position that has the maximum orbit size under W_3, for example $(0, 1, 2) \in R$. The orbit under C_3 is $(0, 1, 2)$, $(1, 2, 0)$, $(2, 0, 1)$, which is obtained by cyclically permuting the coordinates. We place $\mathbf{B}$ at position $(2, 0, 1)$, $\mathbf{C}$ at position $(0, 1, 2)$ and $\mathbf{D}$ at position $(1, 2, 0)$. Since $\mathbf{A}, \mathbf{E} \in \operatorname{cent}_{S_9}(H)$, we will position them each along a different orbit. All remaining positions will be filled with the identity to ensure that we cannot have additional symmetries. We use Proposition 3.16 to ensure aperiodicity. It is easy to see that one gets the required patches by choosing the $2\times2\times2$ cube in the upper right corner from the first and second slices and the other one from the second and third. For this configuration, one obtains $\mathcal{R}(\mathbb{X}_\varepsilon) = \mathbb{Z}^3 \rtimes C_9$.

Remark 3.21 As a generalization of Example 3.20, for any given cyclic groups C_n and C_k, we can construct a substitution ϱ in $\mathbb{Z}^n$, such that $\mathbb{X}_\varrho$ has the symmetry group $\mathbb{Z}^n \times C_k$ and its extended symmetry group is given by $(\mathbb{Z}^n \times C_k) \rtimes C_n$. More precisely, since the extended symmetry group contains an element of order nk, $\mathcal{R}(\mathbb{X}_\varrho) = \mathbb{Z}^n \rtimes C_{nk}$. The substitution can be realized by the following columns:

$$\begin{aligned} \varepsilon_0 &= (a_1\, a_{k+1} \ldots a_{(n-1)k+1}) \ldots (a_k \ldots a_{nk}),\\ \varepsilon_i &= (a_i\, a_{i+1} \ldots a_{k-1+i})(a_{k+i}\, a_{k+i+1} \ldots a_{2k+i-1}) \ldots\\ &\qquad (a_{(n-1)k+i}\, a_{(n-1)k+i+1} \ldots a_{nk-1+i}),\\ \varepsilon_{n+1} &= \mathrm{id}. \end{aligned}$$

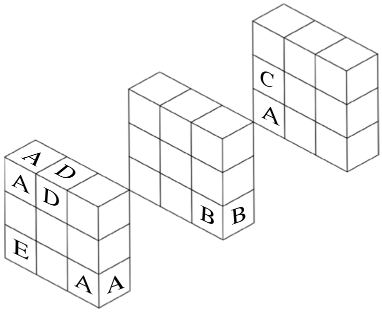


Fig. 7 The letters indicate the respective permutations placed in each cube. The empty cubes are filled with the identity

where i runs from 1 to n, where the values are seen modulo nk. From the columns ε_i with $i \neq 0$ we can see that the centralizer can only be the permutation of the cycles limiting the centralizer to S_k, while ε_0 limits it further to be C_k, since this copy of S_k operates on the cycles independently and the centralizer of a cycle is just the cycle itself. The extended symmetry is realized by the permutation $(a_1 \ldots a_{kn})$ which maps ε_i to ε_{i+1}. Its orbit is determined by the action of $C_n \leq W_n$ on the positioning of the columns.

In the next example we illustrate how important it is to choose compatible structures for the letter-exchange map and the corresponding action in W_d.

Example 3.22 We look at a substitution ϱ on a four-letter alphabet, whose columns generate S_4, thus implying that the subshift has a trivial centralizer; see Theorem 2.8. We plan to have $S_3 \simeq \mathcal{R}(\mathbb{X}_\varrho)/\mathcal{S}(\mathbb{X}_\varrho)$, so we place the columns in a three-dimensional cube; see Fig. 8. As in the previous example, we use the following permutations to build the substitution ϱ:

$$\begin{aligned} \mathbf{A} &= (a\,b\,c\,d), \quad \mathbf{B} = (a\,b\,d\,c), \quad \mathbf{C} = (a\,c\,b\,d), \\ \mathbf{D} &= (a\,c\,d\,b), \quad \mathbf{E} = (a\,d\,b\,c), \quad \mathbf{F} = (a\,d\,c\,b). \end{aligned} \tag{12}$$

The symmetry group is trivial since the columns generate S_4. Conjugation with $\tau = (c\,d)$ maps $\mathbf{A}$ to $\mathbf{B}$, just as any $\tau\kappa$, with $\kappa \in \mathrm{cent}_{S_4}(\mathbf{B})$.

Remark 3.23 The illustration in Fig. 8 contains mostly identity columns for better visibility and to highlight the construction. Being consistent with the first placement, we could fill most positions of the figure non trivially. For our theorems we only require one orbit of identity columns which can always be obtained by looking at powers of the substitution.

Here $C_3 \rtimes C_2 \simeq S_3$ is realized by $(b\,c\,d)(0\,1\,2)$ and $(c\,d)(0\,1)$. The transposition $(c\,d)$ cannot be realized in W_d by mirroring along an axis in the cube since that is not consistent with the interaction between $(b\,c\,d)$ and $(c\,d)$. This can be easily be seen by looking at mirroring along all hyperplanes.

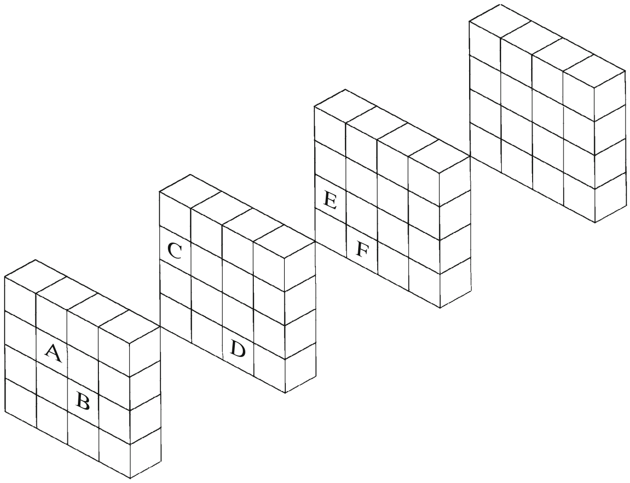


Fig. 8 We illustrate a possible realization with the letters indicating the respective columns. The empty cubes are filled with the identity

$$\begin{tikzcd}
(a\,b\,c\,d)(2,1,0) \arrow[r, shift left, "(b\,c\,d)"] \arrow[r, shift right, "(0\,1\,2)"'] \arrow[d, shift right, "(c\,d)"'] \arrow[d, shift left, "m_{012}"] & (a\,c\,d\,b)(0,2,1) \arrow[d, shift right, "(c\,d)"'] \arrow[d, shift left, "m_{012}"] \\
(a\,b\,d\,c)(1,2,3) \arrow[r, shift left, "(b\,c\,d)"] \arrow[r, shift right, "(0\,1\,2)"'] & (a\,d\,c\,b)/(a\,c\,b\,d)(3,1,2)
\end{tikzcd}$$

We see that the diagram does not commute, thus there is no way to assign a single column to the vertex $(3,1,2)$. One can do this for all axes, which rules out the C_2^3 component in W_3, thus yielding $\mathcal{R}(\mathbb{X}_\varrho) = \mathbb{Z}^d \rtimes S_3$.

Remark 3.24 One can also ask whether, starting with a group H, one can build the centralizer $\mathcal{S}(\mathbb{X}_\varrho)$ and normalizer $\mathcal{R}(\mathbb{X}_\varrho)$ organically from H, under a suitable embedding of H. Consider the Cayley embedding $H \hookrightarrow S_{|H|}$ as in Example 2.12. We know that $\mathrm{cent}_{S_{|H|}}(H) \simeq H$ and $\mathrm{norm}_{S_{|H|}}(H) \simeq H \rtimes \mathrm{Aut}(H)$; see [36]. Since the automorphisms of H are given by conjugation in $S_{|H|}$, they define letter-exchange maps which are compatible with reversors in $\mathcal{R}(\mathbb{X}_\varrho)$. By choosing the dimension appropriately, one can construct a substitution ϱ on $\mathcal{A} = H$ such that the extended symmetry group is given by

$$\mathcal{R}(\mathbb{X}_\varrho) = (\mathbb{Z}^{d(H)} \times H) \rtimes \mathrm{Aut}(H),$$

where we choose $d(H)$ such that $\mathrm{Aut}(H) \leq W_{d(H)}$. This can always be done for $d(H) = |H|$, but depending on $\mathrm{Aut}(H)$, a smaller dimension is possible. Let $\pi \in \mathrm{Aut}(H)$ and let $A_\pi \in W_d$. The construction from the proof of Theorem 3.18 can be applied. Here, the orbits of A_π will not be filled with the same element, but with columns that are determined by π, i.e., $\varrho_{A_\pi(\boldsymbol{i})} = \pi \circ \varrho_{\boldsymbol{i}} \circ \pi^{-1}$, where π is seen as an element of $S_{|H|}$.

These series of examples with more complicated structure can be generalized for arbitrary groups H and P. Here, we have the following version of Theorem 3.18 where the letter exchange map is no longer $\pi = \mathrm{id}$. This means that for these subshifts, the permutations which yield non-trivial symmetries in $\mathcal{S}(\mathbb{X}_\varrho)$ no longer commute with the extended symmetries in $\mathcal{R}(\mathbb{X}_\varrho)$, which accounts for a different semi-direct product structure for $\mathcal{R}(\mathbb{X}_\varrho)$.

Theorem 3.25 *Let H, P be arbitrary finite groups. Then for all $\ell \geq c(P)$, where $c(P)$ is a constant which depends only on the group P, there is a subshift $\mathbb{X}_\varrho$ of an aperiodic, primitive and bijective substitution ϱ such that*

$$\mathcal{S}(\mathbb{X}_\varrho) = \mathbb{Z}^\ell \times H, \qquad \mathcal{R}(\mathbb{X}_\varrho) = (\mathbb{Z}^\ell \times H) \rtimes P.$$

Proof The proof is divided in two parts, beginning with a manual for the construction of the substitution and a second part where we verify the claims made in the construction and check that the subshift has the desired properties. Here we keep in mind that a valid extended symmetry satisfies the conditions in Theorem 3.13, as in Theorem 3.18.

- We first turn our attention to the construction of P which later is supposed to be isomorphic to $\mathcal{R}(\mathbb{X}_\varrho)/\mathcal{S}(\mathbb{X}_\varrho)$. For that purpose we embed $P \hookrightarrow S_\ell$ which is certainly possible for some ℓ. It is clear that there is a minimal $c(P) \in \mathbb{N}$ for which this embedding is possible, and that every $\ell \geq c(P)$ gives a valid embedding as well. This means the choice of ℓ has a lower bound, but can be increased arbitrarily. This chosen ℓ determines the dimension of the space $\mathbb{Z}^\ell$ where the subshift is constructed. Let us now fix a suitable ℓ, excluding $\ell = 2, 3, 6$ since we want to use $\mathrm{Aut}_{S_\ell}(S_\ell) = \mathrm{Inn}_{S_\ell}(S_\ell) \simeq S_\ell$ which does not hold for these values of ℓ; see [35].
- Next, we look for suitable columns for our substitution. Choose the set $T = \{\epsilon_1, \ldots, \epsilon_k\}$ of all transpositions in S_ℓ, together with the identity column as the set of columns. T generates S_ℓ and the action of S_ℓ (viewed as the automorphism group) acts faithfully on T. From this, we get that $P \subset S_\ell \simeq \mathrm{Inn}_{S_\ell}(S_\ell) \subset \mathrm{norm}_{S_\ell}(\{\epsilon_1, \ldots, \epsilon_k\})$. This is enough for now, since $P \subset \mathrm{norm}_{S_\ell}(\{\epsilon_1, \ldots, \epsilon_k\})$ and we can exclude the surplus later.
- Now, we compute the centralizer of the column group. In our current construction the centralizer is trivial, which is why we need to modify our columns. We do this by extending the set $\{a, \ldots, \ell\}$ to $\mathcal{A} = \{a_1, \ldots, a_{|H|}, b_1, \ldots, b_{|H|}, \ldots, \ell_1, \ldots, \ell_{|H|}\}$, which will be our alphabet. We simply duplicate the cycles in each column: The elements of T are embedded into $S_\mathcal{A}$ via $\epsilon_i = (x\ y) \mapsto \varepsilon_i = (x_1\ y_1) \cdots (x_{|H|}\ y_{|H|})$, where $x, y \in \{a, \ldots, \ell\}$.
- We embed $H \hookrightarrow S_{|H|}$ via the usual Cayley embedding. This group only acts on the indices of the letters in the new alphabet. The action on the indices is applied to every $\{a, \ldots, \ell\}$, giving the final set of columns $\{\eta_1, \ldots, \eta_{|H|}\}$ added to the set $\{\varepsilon_1, \ldots, \varepsilon_k\}$, which will be the final set of columns we use in building ϱ. Every η_i is of the form

$$\eta_i = \prod_m (a_m\, a_{\tau(m)}\, a_{\tau^2(m)} \ldots)(b_m\, b_{\tau(m)}\, b_{\tau^2(m)} \ldots) \ldots (\ell_m\, \ell_{\tau(m)}\, \ell_{\tau^2(m)} \ldots),$$

where $\tau \in H$ and where we are multiplying over all orbit representatives m of τ. Here we define $G_\varrho = \langle \varepsilon_1, \ldots, \varepsilon_k, \eta_1, \ldots, \eta_{|H|} \rangle$.
- The Cayley embedding guarantees that $\mathrm{cent}_{S_{\ell|H|}}(G_\varrho) \simeq H$, where $G_\varrho = G^{(1)}$ is the column group of ϱ. We can decrease the size of $\mathcal{R}(\mathbb{X}_\varrho)/\mathcal{S}(\mathbb{X}_\varrho)$ with the same arguments as in Theorem 3.18. This way we achieve a group $\mathcal{R}(\mathbb{X}_\varrho)/\mathcal{S}(\mathbb{X}_\varrho) \simeq P$ where the letter exchange component π of the extended symmetries is not in $\mathrm{cent}_{S_{\ell|H|}}(G_\varrho)$.

Aperiodicity of $\mathbb{X}_\varrho$ can be easily obtained via proximal pairs. Regarding primitivity, it is sufficient to check the transitivity of G_ϱ and use Proposition 2.3. For any pair (x_j, y_k) of letters with indices chosen from the alphabet we need to find a $g \in G_\varrho$ such that $gx_j = y_k$. Note that the permutation $(x_1\, y_1) \ldots (x_j\, y_j) \ldots (x_{|H|}\, y_{|H|}) \in G_\varrho$ and maps x_j to y_j. Now we need to map y_j to y_k, which is an action solely on the indices. The mapping on the indices can be realized by the right embedding copy of H in $S_{|H|}$ and thus by an element composed of the columns $\{\eta_1, \ldots, \eta_{|H|}\}$.

Let us prove that the centralizer is indeed isomorphic to H. The centralizer of $G_{\{\varepsilon_1,\ldots,\varepsilon_k\}}$ can only contain elements that are pure index permutations, since those columns generate S_ℓ, which is diagonally embedded into $S_{\ell|H|}$. Since the structure of the cycles in each column is independent of the index, any index permutation is an element of $\mathrm{cent}_{S_{\ell|H|}}(G_{\{\varepsilon_1,\ldots,\varepsilon_k\}}) = S_{|H|}$.

We continue by determining $\mathrm{cent}_{S_{\ell|H|}}(G_{\{\eta_1,\ldots,\eta_{|H|}\}}) \cap S_{|H|}$. From above, $S_{|H|}$ consists of the pure index switches and since $\eta_1, \ldots, \eta_{|H|}$ are the columns generated by the Cayley embedding of H into $S_{|H|}$ their centralizer is isomorphic to H. This completes the proof that $\mathrm{cent}_{S_{\ell|H|}}(G_\varrho) = H \cap S_{|H|} = H$.

An automorphism $\alpha' \in \mathrm{Aut}_{S_\ell}(\langle T \rangle) = S_\ell$ lifts to an automorphism α on G_ϱ as follows:

$$\text{if} \quad \alpha'(\epsilon_i) = \epsilon_j, \quad \text{then} \quad \alpha(\varepsilon_i) := \varepsilon_j \quad \text{and} \quad \alpha(\eta_i) := \eta_i.$$

Thus $S_\ell \le \mathrm{Inn}_{S_{\ell|H|}}(G_\varrho) \le \mathrm{Aut}_{S_{\ell|H|}}(G_\varrho)$ and hence $P \le \mathrm{Inn}_{S_{\ell|H|}}(G_\varrho)$. Then we can use the geometric placement of the columns in Theorem 3.18 in the substitution to exclude any unwanted W_ℓ-component by setting $\pi \circ \varrho_{\boldsymbol{i}} \circ \pi^{-1} \neq \varrho_{A_\pi \boldsymbol{i}}$ for at least one $\boldsymbol{i} \in R$ whenever $A_\pi \notin P$. The desired symmetries are obtained by positioning the columns such that the previous equation yields an equality, which finishes the proof. □

Remark 3.26 Theorems 3.18 and 3.25 fall under realization theorems for subshifts. The most general current result along this vein known to the authors is that of Cortez and Petite, which states that every countable group H can be realized as a subgroup $H \le \mathcal{R}(\mathbb{X}, \Gamma)$, where $\mathcal{R}(\mathbb{X}, \Gamma)$ is the normalizer of the action of a free abelian group Γ on an aperiodic minimal Cantor space $\mathbb{X}$; see [13].

4 Concluding Remarks

While the higher-dimensional criteria in Theorems 3.13 and 3.11, which confirm or rule out the existence of extended symmetries, are rather general, it remains unclear how to find a way to extend this to a larger (possibly all) class of systems, with no constraints on the geometry of the supertiles. This is related to a question of determining whether, given a substitution in $\mathbb{Z}^d$ (or $\mathbb{R}^d$), one can come up with an algorithm which decides whether there is a simpler substitution which generates the same or a topologically conjugate subshift, which is easier to investigate. This is exactly the case for the two-dimensional Thue–Morse substitution in Fig. 2. Such an issue is non-trivial both in the tiling and the subshift context; see [12,18,25].

Note that the letter-exchange map $\pi \in S_{|\mathcal{A}|}$ in Theorem 3.13 always induces a conjugacy between columns whenever it generates a valid reversor. It would be interesting to know whether outer automorphisms in this case can yield valid reversors for a bijective substitution subshift in $\mathbb{Z}^d$, for example for those whose geometries are not covered by Theorems 3.13 and 3.11. For instance, $\mathrm{Aut}(S_6)$ contains elements which are not realized by conjugation.

Another natural question would be to determine other possibilities for $\mathcal{S}(\mathbb{X}_\varrho)$ and $\mathcal{R}(\mathbb{X}_\varrho)$ outside the class of bijective, constant-length substitutions. Here, the higher-dimensional generalizations of the Rudin–Shapiro substitution would be good candidates; see [20]. There are also substitutive planar tilings with $|\mathcal{R}(\mathbb{X})/\mathcal{S}(\mathbb{X})| = D_6$, which arises from the hexagonal symmetry satisfied by the underlying tiling. For these classes, and in the examples treated above, the simple geometry of the tiles introduces a form of rigidity which leads to $\mathcal{R}(\mathbb{X})$ being a finite extension of $\mathcal{S}(\mathbb{X})$; see [6, Sect. 5] for the notion of hypercubic shifts. There are substitution tilings whose expansive maps Q are no longer diagonal matrices, and whose supertiles have fractal boundaries; compare [22, Ex. 12], which allows more freedom in terms of admissible elements of $\mathrm{GL}(d, \mathbb{Z})$ which generate reversors. This raises the following question:

Question 4.1 What is the weakest condition on the subshift/tiling dynamical system $\mathbb{X}$ which guarantees $[\mathcal{R}(\mathbb{X}) : \mathcal{S}(\mathbb{X})] < \infty$?

This is always true in one dimension regardless of complexity, since either the subshift is reversible or not, but is non-trivial in higher dimensions because $|\mathrm{GL}(d, \mathbb{Z})| = \infty$ for $d > 1$, so infinite extensions are possible; see [3]. We suspect that this is connected to the notions of linear repetitivity, finite local complexity, and rotational complexity; compare [6, Cor. 4] and [25]. For inflation systems, the compatibility condition $[A, Q] = 0$ in Theorem 3.13 might also be necessary in general when the maximal equicontinuous factor (MEF) has an explicit form.

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