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LETTER TO THE EDITOR

A symmetry group of a Thue–Morse quasicrystal

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Abstract. We present a method of coding general self-similar structures. In particular, we construct a symmetry group of a one-dimensional Thue–Morse quasicrystal, i.e. of a nonperiodic ground state of a certain translation-invariant, exponentially decaying interaction.

A symmetry group of a three-dimensional crystal consists of lattice translations, rotations, and reflections. Starting from any point of a crystal, we can reach any other point, successively applying different elements of the symmetry group of the crystal. It was recently shown [1, 2] that certain one-dimensional quasicrystals can be built by successive applications, on one of its points, of elements of certain discrete affine semigroups. Here we describe a general method, based on ideas contained in [3, 4], of representing self-similar structures by one-sided sequences of two symbols. In particular, we construct a symmetry group of a Thue–Morse quasicrystal, i.e. of a nonperiodic ground state of a certain one-dimensional classical lattice-gas model.

In one-dimensional classical lattice-gas models, every site of the lattice \( \mathbb{Z} \) (the set of all integers) can be occupied by a particle or be empty. Configurations of such models are therefore elements of \( \Omega = \{0, 1\}^\mathbb{Z} \), where 1 denotes the presence and 0 denotes the absence of a particle at any given lattice site. By \( X(i) \) we denote the projection of \( X \) to a lattice site \( i \in \mathbb{Z} \).

The Thue–Morse example. We use the Thue–Morse substitution rule to construct a configuration in \( \Omega \). We put 1 at the origin and perform alternatively to the right and to the left the following substitution: \( 1 \rightarrow 10, 0 \rightarrow 01 \). After the first right substitution we obtain 10, which is the configuration on \([0, 1]\), then the substitution to the left gives us 0110 on \([-2, 1]\) (the substitution to the left means that we replace 1 by 01 and 0 by 10), then we obtain 0110101 on \([-2, 5]\) and so on. The effect of performing the substitution to the right or left is the same as taking a sequence of symbols already obtained, changing every 0 to 1 and every 1 to 0 and then placing the new sequence either right or left in relation to the previous sequence.

In this manner we obtain a nonperiodic configuration \( X_{TM} \in \Omega \). Note that if all substitutions were performed to the right, we would obtain the well known one-sided Thue–Morse configuration: \( 10010110100110101 \ldots \) [5–7].

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Let $T$ be a translation operator, i.e. $T : \Omega \to \Omega$, $T(X)(i) = X(i - 1)$, $X \in \Omega$. Let $G_{TM}$ be a closure (in the product topology of the discrete topologies on $\{0, 1\}$) of the orbit of $X_{TM}$ by translations, i.e. $G_{TM} = \{T^n(X_{TM}), n \geq 0\}$. We call elements of $G_{TM}$ two-sided Thue–Morse configurations. It can be shown that $G_{TM}$ supports exactly one translation-invariant probability measure $\mu_{TM}$ on $\Omega$. Such a measure is said to be uniquely ergodic and can be obtained as the limit of averaging over $X_{TM}$ and its translates:

$$\mu_{TM} = \lim_{n \to \infty} \left( \frac{1}{n} \sum_{i=1}^{n} \delta(T^i(X_{TM})) \right),$$

where $\delta(T^i(X_{TM}))$ is the probability measure assigning probability 1 to $T^i(X_{TM})$. It means that all two-sided Thue–Morse configurations look locally identical—any local pattern of particles appears in all of them with the same density (defined uniformly in space). It is also said that such configurations belong to the same isomorphism class.

The Thue–Morse measure is the unique ground state, i.e. a measure supported by configurations with the minimal energy density, of certain exponentially decaying, translation-invariant, four-body interaction [10–12]. Multilayer Thue–Morse superlattice heterostructures were recently made by means of the molecular beam epitaxy and were investigated by Raman scattering [13] and high resolution x-ray diffraction [14]. Nonperiodic order present in Thue–Morse configurations (and in Fibonacci configurations defined below) was investigated in [15–17].

The Fibonacci example. We repeat the above procedure using the Fibonacci substitution:

$0 \to 01$, $1 \to 0$. We put 0 at the origin and apply alternatively the above substitution to the right and left. We obtain the configuration $X_F \in \Omega$. If all substitutions were performed to the right we would get the right one-sided Fibonacci configuration 01001010... Denote by $G_F$ the closure of the orbit of $X_F$ by translations. The elements of $G_F$ are called two-sided Fibonacci configurations. $G_F$ supports the uniquely ergodic measure $\mu_F$ which is the unique ground state of any exponentially decaying, strictly convex, repulsive interaction and a chemical potential which fixes the density of particles to be equal to the square of the golden ratio $(2/(1 + \sqrt{5}))^2$ [18–20].

We shall now discuss a concept of self-similarity. Let $X \in \Omega$. Let us assume that there are two types of finite configurations, we denote them by $s_0$, $s_1$, such that we can group all symbols of $X$ into successive local configurations of these types. We then construct $Y_X \in \Omega$. If all substitutions were performed to the right we would get the right one-sided Fibonacci configuration 01001010... Denote by $G_F$ the closure of the orbit of $X_F$ by translations. The elements of $G_F$ are called two-sided Fibonacci configurations. $G_F$ supports the uniquely ergodic measure $\mu_F$ which is the unique ground state of any exponentially decaying, strictly convex, repulsive interaction and a chemical potential which fixes the density of particles to be equal to the square of the golden ratio $(2/(1 + \sqrt{5}))^2$ [18–20].

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Definition. A set of configurations, $G \subset \Omega$, is self-similar if for some choice of $s_0$, $s_1$, for every $X \in G$, $Y_X \in G$. Then the grouping of symbols of $X$ into local configurations of the type $s_0$ or $s_1$ is also called self-similar.

The following proposition has been proven in [21].

**Proposition 1.** If a self-similar grouping of symbols, into given local configurations $s_0$, $s_1$, of a configuration $X \in \Omega$ from a self-similar set is unique, then $X$ is nonperiodic.

**Proof by contraposition.** Let us assume that $X$ has period $p$. We repeat the process of grouping symbols until $p < \max\{|c_0|, |c_1|\}$, where $c_0, c_1$ are local configurations of $X$ such
that after all successive groupings they are of $s_0$ and $s_1$ type respectively and $|c_0|, |c_1|$ are lengths of their supports. Now we translate $X$ by $p$ lattice units. $X$ does not change. However, $c_0$ and $c_1$ overlap with their translates. The translation therefore produces a different grouping.

The Thue–Morse example. The set $G_{TM}$ of two-sided Thue–Morse configurations is self-similar and a corresponding self-similar grouping is the following $s_0 = 01 \rightarrow 0, s_1 = 10 \rightarrow 1$.

The Fibonacci example. The set $G_F$ of two-sided Fibonacci configurations is self-similar and a corresponding self-similar grouping is the following $s_0 = 01 \rightarrow 0, s_1 = 0010 \rightarrow 01, s_2 = 0000 \rightarrow 000000$.

We now present a method of coding self-similar sequences.

Let $G \subseteq \Omega$ be a self-similar set and let $X \in G$. If $X(0) = 1$, then we set $C_X(-1) = 1$; if $X(0) = 0$, then $C_X(-1) = 0$. If $0 \in \mathbb{Z}$ belongs to the support of $s_j$, then $C_X(0) = j$. Now we group the symbols of $X$ and construct $Y_X$. If 0 belongs to the support of $s_j$ of $Y_X$, then $C_Y(1) = j$. We group the symbols of $Y_X$, construct $Y_{Y_X}$ and obtain $C_Y(2)$. We continue this procedure infinitely many times and obtain a sequence $C_X(i), -1 \leq i < \infty$. $C_X$ can be seen as an element of a direct product $\mathcal{W} = \bigotimes_{i=0}^{\infty} \mathbb{Z}_2$, where $\mathbb{Z}_2$ is the group of two elements, 0 and 1, with the addition modulo 2 as a group action.

The Fibonacci example. The Fibonacci configurations are represented by elements of $\mathcal{W}_F = \{ W \in \mathcal{W}, W(i)W(i+1) = 0, \text{ for every } i \geq -1 \}$. This restriction on $W$’s is present in a corresponding representation of Penrose tilings [3, 4].

If $C_X \in \mathcal{W}_F$ has both infinitely many 0’s and 1’s, then $X$ is a two-sided Fibonacci configuration, i.e. an element of $G_F$. Otherwise, $X$ is a one-sided Fibonacci configuration. For example, $(0010101010\ldots)$ represents $X_F$ and $(0000000\ldots)$ represents the right one-sided Fibonacci configuration.

The Thue–Morse example. It is easy to see that every element of $\mathcal{W}$ represents either a two-sided Thue–Morse configuration, i.e. an element of $G_{TM}$ or a one-sided Thue–Morse configuration. For example, $(11001100\ldots)$ represents $X_{TM}$, $(11111\ldots)$ represents the right one-sided Thue–Morse configuration (with 1 at the origin) and $(101010\ldots)$ represents the left one-sided Thue–Morse sequence $\ldots 01101001$ (with 1 at the origin) obtained by successive applications of the Thue–Morse substitution to the left. Let us note that the representation of the last configuration has infinitely many 0’s and 1’s. However, we would like to represent one-sided configurations by sequences with either finitely many 0’s or finitely many 1’s. To achieve this, we represent Thue–Morse configurations in another way.

Observe that every Thue–Morse configuration can be obtained by successive applications of the Thue–Morse substitution either to the right or to the left. If $X(0) = 1$, then let $C_X'(1) = 1$; if $X(0) = 0$, then let $C_X'(0) = 0$. We put $C_X'(i) = 1$ if the $i$th substitution was performed to the right and $C_X(i) = 0$ if the $i$th substitution was performed to the left. Such $C_X'$ is again an element of $\mathcal{W}$.

Now, the right one-sided Thue–Morse configuration is still represented by $(111111\ldots)$ but the left one is represented by $(100000\ldots)$ and $X_{TM}$ by $(1101010\ldots)$. It is easy to see that $C_X'(i) = (C_X(i-1) + C_X(i) + 1) \mod 2$. $X \in G_{TM}$ if and only if $C_X'$ has both infinitely many 0’s and 1’s.
Obviously, for some of the elements of $W$, corresponding Thue–Morse configurations are related by translations, reflections or the transformation changing every 0 to 1 and every 1 to 0. We say that such Thue–Morse configurations are equivalent. Let $U \subset W$ be a subgroup of $W$ consisting of sequences with finitely many 1’s or finitely 0’s. We have the following theorem.

**Theorem 1.** Equivalent classes of Thue–Morse configurations are represented by elements of the coset group $W/U$.

**Proof.** (a) Let $X_1, X_2 \in GT_M$ be related by a translation $T^n$. We group successive symbols of $X_1$ and $X_2$ into $s_0$ and $s_1$ configurations, then we group symbols of $Y_{X_1}$ and $Y_{X_2}$. We repeat grouping until, say in the $i$th grouping, we obtain for both $X_1$ and $X_2$ the local configurations of the same type, either $s_0$ or $s_1$, with supports containing both the origin and $n$ (they are related by the same translation as $X_1$ and $X_2$). It follows that $C'_{X_1}(j) = C'_{X_2}(j)$, for every $j > i$ and therefore $C'_{X_1} = C'_{X_2} + U$, where $U(j) = 0$ for $j > i$.

Conversely, let $C'_{X_1} = C'_{X_2} + U$, where $U(j) = 0$ for $j > i$. Let $c(k)$ be a local configuration obtained by successive applications of substitutions corresponding to $C'_{X_k}(l), l \leq i, k = 1, 2$. If $c(1)$ and $c(2)$ are related by a translation, then $X_1$ and $X_2$ are related by the same translation. If $c(1)$ and $c(2)$ are related by a translation and the interchanging of 0’s and 1’s, then $X_1$ and $X_2$ are related by the same translation and the interchanging of 0’s and 1’s. Observe that the first situation occurs if the absolute value of the difference of the number of 1’s in $C'_{X_k}(l)$ and $C'_{X_2}(l), l \leq i$, is even, otherwise we have the second case.

(b) $X_1, X_2 \in GT_M$ are related by the interchanging of 0’s and 1’s if and only if $C'_{X_1} = C'_{X_2} + (10000\ldots)$. (c) $X_1, X_2 \in GT_M$ are related by the reflection around the origin if and only if $C'_{X_1} = C'_{X_2} + (01111\ldots)$. □

Let us note that the above group acts on the whole set $G_{TM}$ of the Thue–Morse configurations. We shall now construct a symmetry group which leaves every Thue–Morse configuration invariant. This corresponds to crystal symmetries mentioned at the very beginning of the paper.

**A symmetry group of the Thue–Morse configurations.** The following theorem gives us the positions of particles, i.e. 1’s in a Thue–Morse configuration.

**Theorem 2.** Let $X$ be a Thue–Morse configuration, with 1 at the origin, and represented by $C'_{X} \in W$. We have

$$X(i) = 1 \iff i = \sum_{k=0}^{\infty} (-1)^{(1+C'_{X}(k))} 2^k a_k$$

where $a_k \in \{0, 1\}, k \geq 0$ and in the sum there are finite and even numbers of nonzero terms.

**Proof.** Let us recall that the effect of performing the substitution to the right or to the left is the same as taking a sequence of symbols already obtained, changing every 0 to 1 and every 1 to 0 and then placing the new sequence right to or left to the previous sequence. We call such sequences blocks. If we start with 1 at the origin, then every second block
placed right to or left to the previous block begins with 1. Let \( X(i) = 1 \). We identify the first block containing the origin to which \( i \) belongs and call it the exterior block. If \( i \) is not at the beginning of this block, we then have to find out to which one of the two subblocks it belongs. We continue this procedure until we identify the block such that \( i \) is at the beginning of it. If the exterior block begins with 1, then its position is given by the sum in (1) with an even number of nonzero terms and then we have to identify an even number of additional subblocks; to obtain (1) we have to add to the position of the left end of the exterior block an even number of different powers of 2. In the other case, the exterior block begins with 0 and its position is given by the sum in (1) with an odd number of nonzero \( a_i \)'s, but we have to identify an odd number of additional subblocks. For example, in the right one-side Thue–Morse sequence represented by (1111111...), all exterior blocks begin with 1 at the origin.

Denote by \( S_{TM} \) the set of all sequences \( \{a_i, i \geq 0\} \) such that \( a_i = 1 \) for finite and even number of \( i \)'s and otherwise \( a_i = 0 \). \( S_{TM} \) is a subgroup of \( \otimes_{i=0}^{\infty} \mathbb{Z}_2 \). It is generated by an infinite number of elements (with two successive \( 1 \)'s and \( 0 \)'s otherwise). A Thue–Morse quasicrystal is generated by successive applications of elements of \( S_{TM} \) to the particle at the origin.

More precisely, positions of particles in a two-sided Thue–Morse configuration \( X \in G_{TM} \) is a subset \( \mathbb{Z}_X \subset \mathbb{Z} \). The coding of \( X \), \( C_X \), gives us an addition, \( +_X \), in \( \mathbb{Z}_X \), such that \((\mathbb{Z}_X, +_X)\) is a group.

For example, \( \mathbb{Z}_{XTM} \) is generated by \( \{(-1)^k+2^k : k \geq 0\} \).

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